

## Physical Chemistry Research Articles Published in the Bulletin of the Korean Chemical Society: 2003-2007

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*Received January 14, 2008*

The physical chemistry (PC) articles published in the *Bulletin of the Korean Chemical Society* (BKCS) from 2003 to 2007 are surveyed, and in-depth content analysis was conducted to classify the PC articles into 12 topics used in *The Journal of Physical Chemistry* (JPC). The PC articles published in the *Journal of the American Chemical Society* (JACS) in 2007 are also surveyed. The extensive summary of all PC articles in BKCS for the last five years reveals the current trend of physical chemistry research in Korea. The comparison study with the JACS shows that the proportion of PC articles among all articles published in BKCS (16%) is slightly higher than that of JACS (11%), and the non-Korean authorship ratio of BKCS (12%) is very low compared with the non-US authorship of JACS (52%). From the comparison study with articles published in JPC in 2007, it is found that BKCS disseminates various topics of physical chemistry researches adequately. In particular, BKCS most frequently published PC articles in molecular structure and spectroscopy topics, whereas JPC published surface chemistry and nano-chemistry articles most frequently. It is concluded that BKCS should publish more articles to be a leading journal, and it is suggested that the SCI impact factor of BKCS must be increased by improving the electronic version of BKCS.

**Key Words :** Physical chemistry, Bulletin of the Korean Chemical Society, Journal of the American Chemical Society, The Journal of Physical Chemistry

### Introduction

The *Bulletin of the Korean Chemical Society* (BKCS) publishes original chemical research works for all fields of chemistry in the form of accounts, communications, notes, and articles.<sup>1</sup> (The four forms of publications will be called "articles" throughout this work.) The executive editorial board of BKCS consists of an editor-in-chief, an editor, and 12 associate editors. The 12 associate editors handle the 11 chemistry fields which are "Analytical chemistry", "Electrochemistry", "Industrial chemistry", "Inorganic chemistry", "Life-science chemistry", "Macromolecular chemistry", "Medicinal chemistry", "Non-synthetic organic chemistry", "Organic synthesis (2 associate editors assigned)", "Physical chemistry", and "Material chemistry". This work concentrates only on "physical chemistry articles (PC articles)" published in BKCS from the year of 2003 through 2007. Thus, articles submitted to the associate editor who is in charge of "Physical chemistry" are automatically counted as the PC articles. In addition, articles (for example, an account) submitted to the editor-in-chief or to the editor are examined by the authors of this work and those articles judged as PC articles are included in the study.

Research contents presented in the PC articles of BKCS are summarized. The summary is given in the order of "physical chemistry topics" adopted in *The Journal of Physical Chemistry* (see below.) Although the summary is not a review of physical chemistry researches in Korea, it may reveal the research level and research interests pre-

sented in BKCS. Through this summarization one may understand the current trend of physical chemistry researches in Korea.

BKCS is compared with the *Journal of the American Chemical Society* (JACS),<sup>2</sup> and with *The Journal of Physical Chemistry* (JPC) in a quantitative way. JACS contains articles in all fields of chemistry. Thus the PC articles are selected by the authors. The survey year for JACS is the year of 2007 only. The JPC consists of three separate journals, A, B, and C.<sup>3</sup> All articles in the three JPC journals are counted as PC articles. Since JPC publishes PC articles in 12 categories of "topics", the authors classify the PC articles in BKCS into the 12 topics correspondingly. It makes the comparison of distribution of articles among 12 topics of physical chemistry between BKCS and JPC. The survey year for JPC is also the year of 2007 only.

Through the scientometric analyses on the PC articles in BKCS and through the comparison of such data with JACS and with JPC, the problems that may reside in BKCS are examined. Finally the future direction that BKCS should pursue to be a leading journal is suggested.

It is advised that a potential reader, before reading the main text, should scrutinize the Table 1 that contains the terminology used in this work.

### Physical Chemistry Researches in BKCS

From 2003 to 2007, there are 346 PC articles published in BKCS. (See Table 2) To understand the current trend of

**Table 1.** Abbreviations and Glossary

Terms	Explanations
BKCS	<i>Bulletin of the Korean Chemical Society</i> published by the Korean Chemical Society for the purpose of rapid distribution of research information in the field of pure and applied chemistry to the chemical community worldwide. From 2003 to 2007, 12 issues (No. 1-12) are published each year.
JACS	<i>Journal of the American Chemical Society</i> published by the American Chemical Society. It is the venue for the publication and broad dissemination of fundamental research in all of chemistry, both in the core areas and at the interface of chemistry and biology, neurochemistry, materials, and single molecule chemistry. In 2007, 51 issues (No. 1-51) have been published.
JPC	<i>The Journal of Physical Chemistry</i> published by the American Chemical Society. In 1997, this journal was divided into two separate journals, <i>The Journal of Physical Chemistry A</i> and <i>B</i> . Currently (from the year of 2007) it consists of three separate journals, i.e., <i>The Journal of Physical Chemistry A</i> , <i>The Journal of Physical Chemistry B</i> , and <i>The Journal of Physical Chemistry C</i> .
JPC A	<i>The Journal of Physical Chemistry A</i> published by the American Chemical Society. It covers research topics of physical chemistry including dynamics, clusters, excited states, kinetics, spectroscopy, atmospheric, environmental and green chemistry, molecular structure, quantum chemistry, and general theory. In 2007, 51 issues (No. 1-51) have been published.
JPC B	<i>The Journal of Physical Chemistry B</i> published by the American Chemical Society. It covers research topics of physical chemistry of condensed matter including macromolecules, soft matter, surfactants, membranes, statistical mechanics, thermodynamics, medium effects, and biophysical chemistry. In 2007, 51 issues (No. 1-51) have been published.
JPC C	<i>The Journal of Physical Chemistry C</i> published by the American Chemical Society. It covers research topics of physical chemistry including nanoparticles and nanostructures, surfaces, interfaces, catalysis, electron transport, optical and electronic devices, and energy conversion and storage. The journal was launched in the year of 2007 and 51 issues (No. 1-51) have been published.
Publication years of journals under survey	BKCS : All issues of year 2003-2007 (Vol. 24-28) JACS : All issues of year 2007 (Vol. 119) JPC A, B, C : All issues of year 2007 (Vol. 111)
Article	All types of published research papers in the Journals of interest. It includes 'communications', 'notes', 'letters', 'reviews', 'accounts', and genuine 'articles'. 'Editorials', 'comments', and 'book reviews' are excluded.
PC Article	'Physical Chemistry Article'. Articles whose main theme contains a research topic frequently studied in physical chemistry. All the articles published in JPC are considered as PC articles. For BKCS and JACS, each article is read by the authors and consequently classified as PC article or not. The authors' bias may enter in this process.
Topic	The research topics listed in JPC A, B, and C are reorganized into 12 topics of physical chemistry. (The list of 12 topics is provided in Table 4.) The topic of an article is not explicitly shown in BKCS and JACS, therefore the authors read the article and assign an appropriate topic to it. The authors' bias may enter in this process.
Korean authorship	When at least one of authors in an article has a Korean address, the article is classified as one having a Korean authorship. When an article has both of Korean and USA addresses, it is counted as a Korean article in BKCS but as a US article in JACS. An article that does not have a Korean authorship is called 'Non-Korean article'.
US authorship	When at least one of authors in a JACS article has a USA address, the article is classified as one having a US authorship.
SCI journal	The scientific journals listed in Science Citation Index (SCI) and Science Citation Index Expanded (SCI-E) published by The Thomson Scientific.

physical chemistry researches, the contents of the PC articles are listed. The researches in BKCS are classified into 12 topics of JPC for the convenience of presentation. (See the next section.) The authors do not intend to cite all the PC articles published in BKCS, yet some articles are presented as examples.

**Dynamics, Clusters, Excited states:** Quasiclassical and quantum mechanical collision dynamics calculations for various chemical systems are presented. The nonadiabatic transitions among the five lower states in the photodis-

sociation of Cl<sub>2</sub>, Br<sub>2</sub>, and I<sub>2</sub> are studied by using the spin-orbit configuration interaction method and the semiclassical time-dependent coupled Schrödinger equations.<sup>4</sup> Vibrational predissociation dynamics of I<sub>2</sub>(B)-Ne is quantum mechanically studied.<sup>5</sup> Relationships between charge transfer mechanism and quantum coherence are investigated through a real-time quantum dynamics approach.<sup>6</sup> The reaction probability and cross section for N(<sup>4</sup>S) + O<sub>2</sub>(X<sup>3</sup>Σ<sub>g</sub><sup>-</sup>) → NO(X<sup>2</sup>Π) + O(<sup>3</sup>P) reaction are calculated by using the quasiclassical trajectory method.<sup>7</sup>

The classical trajectory calculations are also reported. For example, the collision-induced intramolecular energy flow in vibrationally excited toluene in the collision with HF is studied.<sup>8-10</sup> The reaction of methyl radical with iodine molecule on an attractive potential energy surface, the reaction of gas-phase hydrogen atoms with H atoms chemisorbed on a graphite surface, and the vibrational relaxation and competitive C-H bond dissociations in vibrationally excited methylpyrazine in the collision with HF are all studied by using the classical trajectory procedures.<sup>11-13</sup>

Structural dynamics and photodissociation dynamics are frequently investigated spectroscopically. For example, structural dynamics of myoglobin is probed by femtosecond infrared spectroscopy of the amide band.<sup>14</sup> The photodynamics of 1-hydroxyanthraquinone and 1-deuterioanthraquinone is investigated in toluene with time-resolved emission and femtosecond transient transmittance techniques.<sup>15</sup> The excitation energy transfer rates of various forms of multiporphyrin arrays are determined by time-resolved spectroscopic measurements.<sup>16</sup> The photoexcitation dynamics of *S*-nitrosoglutathione is probed by femtosecond mid-IR spectroscopy.<sup>17</sup> The photodissociation dynamics of formic acid, cyanamide, and *tert*-butyl isocyanide is investigated by analyzing laser induced fluorescence spectra.<sup>18-20</sup>

For cluster researches, recent experimental and theoretical advances on the aromatic alcohol-water clusters are reviewed.<sup>21</sup> The structures of various clusters, *e.g.*, alkane clusters in a mesoscopic solvent, acetonitrile-water clusters, proline-water clusters and anthracene anion tetramers, are theoretically determined.<sup>22-26</sup> Experimentally the temperature dependent structures of electron-water clusters and yttrium oxide cluster formation are investigated.<sup>27,28</sup> Formation of silver cluster ions in MALDI is studied.<sup>29</sup> Some researches involving cluster reactions, *e.g.*, intracluster ion-molecule reactions of  $\text{Ti}^+(\text{H}_2\text{O})_n$ ,  $\text{Ti}^+(\text{CH}_3\text{OCH}_3)_n$ , and  $\text{Ti}^+(\text{CH}_3\text{OD})_n$  complexes and proton transfer in  $\text{HOCl} + \text{HCl}$  and  $\text{H}_2\text{O} + \text{ClONO}_2$  on water clusters, are reported.<sup>30,31</sup>

For excited-state dynamics, the excited-state intramolecular proton transfers of 1-hydroxyanthraquinone, 2-(2'-hydroxyphenyl)benzoxazole derivatives, and 1,5- and 1,8-dihydroxyanthraquinones adsorbed onto  $\text{SiO}_2$ ,  $\text{SiO}_2\text{-Al}_2\text{O}_3$ , and  $\text{Al}_2\text{O}_3$  matrices are either spectroscopically or theoretically investigated.<sup>32,34</sup>

**Kinetics, Spectroscopy:** Kinetics and mechanism study is one of the most frequently reported physical chemistry topics in BKCS. The research subjects are the addition of benzylamines to benzylidene Meldrum's acids in acetonitrile,<sup>35</sup> the aminolysis of phenacyl bromides in acetonitrile,<sup>36</sup> the pyridinolysis of aryl phenyl isothiocyanophosphate in acetonitrile,<sup>37</sup> the hydrolysis of *N*-benzoyl-4,5-diphenylimidazole derivatives,<sup>38</sup> the hydrolysis reactions of *N*-heteroaryl-4(5)-nitroimidazoles,<sup>39</sup> the aminolysis of anilino thioethers with benzylamines in acetonitrile,<sup>40</sup> the cleavage of *N*-methylphthalamic acid in mixed acidic aqueous-acetonitrile solvent,<sup>41</sup> and the addition of benzylamines to  $\alpha$ -phenyl- $\beta$ -thiophenylacrylonitriles in acetonitrile.<sup>42</sup> Reaction rates or rate constants are determined for a few

systems, for example, conversion of  $\text{CO}_2$  to CO with  $\text{CH}_4$  over  $\text{Ni/SiO}_2$ , proton transfer reactions and ion-molecule reactions of bifunctional ethanes of  $\text{H}_2\text{NCH}_2\text{CH}_2\text{NH}_2$ ,  $\text{H}_2\text{NCH}_2\text{CH}_2\text{OH}$ , and  $\text{OHCH}_2\text{CH}_2\text{OH}$ , the ionic micellar-mediated semi-ionic bimolecular reaction, and bimolecular reactions of O(<sup>3</sup>P) atom with  $\text{SiH}_4$  and  $\text{SiHCl}_3$ .<sup>43-46</sup> Solvolyses of 3,4-dimethoxybenzenesulfonyl chloride in various aqueous mixtures are also studied.<sup>47</sup>

Other kinetics studies are, for example, diffusion-influenced kinetics of reactions involving polymers,<sup>48</sup> photochemical reaction of nalidixic acid in methanol,<sup>49</sup> kinetics of bromophenol blue fading,<sup>50,51</sup> and acid catalyzed reactions of sulfenamides.<sup>52</sup> The kinetics nature of the following reactions, *e.g.*, the Belousov-Zhabotinsky reaction,<sup>53,54</sup> unimolecular dissociation reaction,<sup>55,56</sup> ignition reaction,<sup>57</sup> inhibition reaction,<sup>58</sup> oscillating reaction,<sup>59</sup> and radical reaction,<sup>60</sup> is also investigated.

New spectroscopic methods, new theoretical interpretations, improvements of current spectroscopic technique, and design or building of spectroscopic instruments are suggested. Coherent multidimensional vibrational spectroscopy is introduced.<sup>61</sup> Theoretical descriptions of two-dimensional vibrational and electronic spectroscopy are presented.<sup>62</sup> Principal component analysis based two-dimensional correlation spectroscopy is described.<sup>63</sup> Femtosecond stimulated Raman spectroscopy is developed.<sup>64</sup> The light pressure force from an optical standing wave is used to focus an atomic beam to submicrometer dimensions.<sup>65</sup> A description and demonstration of homodyne-detected two-color transient grating signal are presented.<sup>66</sup> Two different electronically resonant two-dimensional spectroscopies are described.<sup>67</sup> Theoretical nonlinear response functions are suggested.<sup>68</sup> New routes to the preparation of silver-doped sol-gel films for surfaced enhanced Raman scattering (SERS) are found.<sup>69</sup> Various activated-ion electron capture dissociation methods are compared.<sup>70</sup> The well-resolved vibronic emission spectra of the jet-cooled *m*-tolunitrile and *o*-tolunitrile are recorded in the UV region by using a Fourier transform spectrometer.<sup>71,72</sup> A new analytical application of XPS to the identification of organic molecules in room temperature ionic liquid is reported.<sup>73</sup> A pulsed mixing source for bimolecular reaction is developed.<sup>74</sup> A miniaturized time-of-flight mass spectrometer with an electron impact ionization source and sheet membrane introduction is developed.<sup>75</sup> An improved tandem time-of-flight mass spectrometer for photodissociation of ions generated by matrix-assisted laser desorption ionization (MALDI) is constructed.<sup>76</sup> Highly sensitive fluorescence probes for organic vapors are demonstrated.<sup>77</sup> A quadrupole ion trap time-of-flight mass spectrometer to study photo-induced dissociation of biologically important molecules in the gas phase is constructed.<sup>78</sup>

The spectroscopic methods are applied to a vast number of chemical systems. The application researches are listed with a spectroscopic method in a parenthesis. The authors understand that the listed researches may belong to a topic other than the current 'spectroscopy' topic. The subjects studied with spectroscopy are, for example, the methyl

radical recombination following photodissociation of CH<sub>3</sub>I (Time-resolved Photothermal Spectroscopy),<sup>79</sup> the pathway for the thermal imidization of poly(amic acid) (2-D Raman Correlation Spectroscopy),<sup>80</sup> the optical properties of oxotitanium(IV) meso-tetrakis(4-sulfonatophenyl)porphyrin intercalated into the layered double hydroxides (Laser Spectroscopy),<sup>81</sup> quinomethionate adsorbed on silver colloids (SERS),<sup>82</sup> Zn(II)porphyrin using chirped ultrashort pulses (Femtosecond Coherent Spectroscopy),<sup>83</sup> the concentration-dependent IR spectra of urea aqueous solution (2-D Correlation Spectroscopy),<sup>84</sup> the samarium(III) thiodiglycolate complexes (Laser-induced Luminescence),<sup>85</sup> photolysis of Cr(CO)<sub>6</sub> vapor in He or Ar and reactions of Cr atoms with O<sub>2</sub> and N<sub>2</sub>O (UV),<sup>86</sup> characterization of Raman spectra of size-selected TiO<sub>2</sub> nanoparticles (2-D Raman Correlation Spectroscopy),<sup>87</sup> complexation of cesium ion by *p*-tert-butylcalix[6]arene ethyl ester (NMR),<sup>88</sup> optical emission studies of a plume from a graphite target in a nitrogen atmosphere (Laser Ablation),<sup>89</sup> the coordination structure of Zn(II) bound lysine ternary complexes (Tandem MS),<sup>90</sup> fragmentations and proton transfer reactions of mono-, di-, and triethanolamines (FTMS).<sup>91</sup> Substitution effect of anthraquinone (SERS),<sup>92</sup> methyl red adsorbed on untreated and pretreated alumina and silicaalumina (FT Raman),<sup>93</sup> the enhancing effect of organic substances on hydroxyl radical generation during ozonation of water (ESR),<sup>94</sup> poly([ethylene-co-vinyl acetate]-*graft*-vinyl chloride) in solution (NMR),<sup>95</sup> the <sup>1</sup>H and <sup>13</sup>C chemical shifts of flavone and its five derivatives (2-D NMR),<sup>96,97</sup> vibronic relaxation in methyl substituted benzyl radicals (Laser),<sup>98</sup> the fragmentation patterns and ion-molecule reactions of two alkyne alcohols (FTMS),<sup>99</sup> the coil effects on the intermolecular structure of a rod-coil liquid crystalline oligomer (Raman),<sup>100</sup> the dielectric study of methyl acrylate-alcohol mixtures (Reflectometry),<sup>101</sup> the spectrum of CH<sub>4</sub> gas plasma,<sup>102</sup> encapsulation of 6-hydroxyquinoline in heptakis(2,6-di-*o*-methyl)- $\beta$ -cyclodextrin (NMR, UV-VIS),<sup>103</sup> the quenching of ofloxacin, flumequine, and norfloxacin fluorescence by Cu<sup>2+</sup>, Ni<sup>2+</sup>, Co<sup>2+</sup> and Mn<sup>2+</sup> in an aqueous solution (Fluorescence),<sup>104,105</sup> effects of transverse magnetic field on C<sub>2</sub> and CN molecules produced by laser ablation of a graphite target in nitrogen atmosphere (Optical Emission Spectrometry),<sup>106</sup> the photophysical properties of dansyl-*N*-methylaminobenzoic acid as a ligand and its lanthanide-cored complexes (IR),<sup>107</sup> electric field-induced charge transfer of (Bu<sub>4</sub>N)<sub>2</sub>[Ru(dcbpyH)<sub>2</sub>(NCS)<sub>2</sub>] on gold, silver, and copper electrode surfaces (SERS),<sup>108</sup> the energy transfer in allophycocyanin (Raman),<sup>109</sup> singlet oxygen production from different reaction pathway, using solid inorganic peroxides as starting materials,<sup>110</sup> intermolecular electron-transfer dynamics of trans-bis(ferrocene-carboxylato)(tetraphenyl-porphyrinato)titanium(IV) (Time-resolved Laser Spectroscopy),<sup>111</sup> and characterization of synthetic polyamides (MALDI-TOF MS).<sup>112</sup>

**Atmospheric, environmental and green chemistry:** On this topic, there are no articles published in BKCS.

**Molecular structure, Quantum chemistry, General theory:** Theoretical studies of molecular structures by *ab*

*initio* methods or density functional theory constitute a bulk of physical chemistry researches in BKCS. The *ab initio* calculation studies (using the self-consistent field, perturbation theory, configuration interaction, coupled cluster method, G3, etc.) are, for example, intramolecular vibrational frequencies and the hydrogen-bond length in a variety of *N*-methylacetamide-H<sub>2</sub>O complexes,<sup>113</sup> the hydrogen bonding in acetonitrile-water clusters,<sup>114</sup> the nucleophilic substitution reactions of cyclopentadienyl halides,<sup>115</sup> the spin-orbit coupling of SiH, SiH<sup>+</sup>, and SiH<sup>2+</sup>,<sup>116</sup> the structures and energies of BH<sub>5</sub>,<sup>117</sup> positronium atoms using frozen Gaussian-type geminals,<sup>118</sup> the conformational characteristics of the tetramethoxycalix[4]arenes,<sup>119</sup> the structures and complexation energies of penta-*O*-*tert*-butyl ester of *p*-*tert*-butylcalix[5]-arene toward a series of alkyl ammonium guests,<sup>120</sup> the conformational characteristics of the tetraethyl and triethyl ester of *p*-*tert*-butylcalix[4]arene,<sup>121</sup> the hydride ion affinities of carbocations,<sup>122</sup> intersystem electron-transfer in dihydrated iodide anion,<sup>123</sup> potential energy surfaces for the reaction Al + O<sub>2</sub> → AlO + O,<sup>124</sup> the structure of *N*-nitrosoazetidine-2-carboxylic acid,<sup>125</sup> the geometrical parameters, vibrational frequencies, and relative energies of H<sub>2</sub>(A<sub>*n*+1</sub>X<sub>2*n*</sub>)H<sub>2</sub> (A=C, Si; X=O, S; *n* = 1-2) oligomers,<sup>126</sup> the structures and energies of the unimolecular decomposition of methacrylonitrile,<sup>127</sup> the stationary point structures and relative energies between them as well as binding energies of (CO)<sub>2</sub>,<sup>128</sup> the relaxed torsional potential of a liquid crystalline polymer containing an ester functional group in a mesogenic unit,<sup>129</sup> conformations, chemical reactivities and spectroscopic characteristics of some di-substituted ketenes,<sup>130</sup> interpretation of scanning tunneling microscope and atomic force microscope images,<sup>131</sup> the basis set limit binding energy of hydrogen-bonded complexes,<sup>132</sup> the combined *ab initio* and vibrational predissociation spectroscopic studies on methylammonium-(water)<sub>4</sub> complex,<sup>133</sup> the benzene complexes with dimethyl sulfur and fluorinated dimethyl sulfur,<sup>134</sup> the structures, energetics and transfer integrals of the acene tetramers up to pentacene,<sup>135</sup> the characteristic effects of 4,5-disubstituted pyridazin-3-one derivatives with various functional and substituent groups,<sup>136</sup> and the supercritical CO<sub>2</sub> stability of organophosphorous molecules.<sup>137</sup>

Density functional theory (DFT) is also frequently used in computational chemical researches. The DFT researches are, for example, the effects of different polarization conditions on vibrational echo signals for the rigid cyclic dipeptide,<sup>138</sup> the structural and bonding aspects of ( $\eta^5$ -C<sub>5</sub>H<sub>5</sub>)(CO)<sub>2</sub>M≡ER (M=Cr, Mo, W; E=Si, Ge, Sn, Pb; R=terphenyl groups),<sup>139</sup> the lowest energy structure of (H<sub>2</sub>O)<sub>11</sub>,<sup>140</sup> the electron affinity of polychlorinated dibenzo-*p*-dioxins,<sup>141</sup> the reaction mechanism of the pyrolysis of sulphonyl oximes in the gas phase,<sup>142</sup> the structures and gas-phase ionization energies of Meldrum's acid and related cyclic and acyclic compounds,<sup>143</sup> the cubic and quartic anharmonic force field of malonaldehyde,<sup>144</sup> the molecular structure and conformational behavior of 1-hexyl-3,4-dimethylpyrrole and the oligomers up to trimer,<sup>145</sup> the complexation characteristics of tetramethyl and tetraethyl esters of *p*-*tert*-butylcalix[4]arene with

alkali metal cations,<sup>146</sup> the rearrangement of CH<sub>3</sub>SNO<sub>2</sub> to CH<sub>3</sub>SONO,<sup>147</sup> molecular geometries for the cationic and neutral species of OXO (X=Cl, Br, I),<sup>148</sup> the ring-opening reactions of Li<sup>+</sup>-(ethylene carbonate) and Li<sup>+</sup>-(vinylene carbonate),<sup>149</sup> the equilibrium geometries, electronic structures, and energies of borocarbon clusters,<sup>150</sup> the gas phase proton affinity, basicity, and pK<sub>a</sub> values for nitrogen containing heterocyclic aromatic compounds,<sup>151</sup> the structures and complexation energies of *p*-*tert*-butylcalix[6](aza)cryptand with a series of alkylammonium cations,<sup>152</sup> the metal ion-(Gly-Gly-His) complexes,<sup>153</sup> the structures and conformations of *ortho*-, *meta*-, and *para*-methyl red upon proton gain and loss,<sup>154</sup> intermediate complexes in S<sub>N</sub>2 reaction of [Na<sup>+</sup>, F<sup>-</sup>, H<sub>2</sub>O, CH<sub>3</sub>Cl] system,<sup>155</sup> the zinc complexes of DNA bases,<sup>156</sup> complexes of trimethyl ether of monodeoxycalix[4]arene with potassium ion,<sup>157</sup> the water-assisted intramolecular proton transfer in the tautomers of thymine radical cation,<sup>158</sup> the structure, atomic charges and natural bond orbital,<sup>159</sup> the bis(crown-ether) analogue of Troger's base complexed with bisammonium ions,<sup>160</sup> the hydrolyses of dimethylchlorothiophosphate,<sup>161</sup> the structures and proton transfer barriers in proton-bound homodimers of aromatic molecular bases,<sup>162</sup> the molecular structures of the ground and lowest triplet states of 2,3-diazabicyclo[2.2.1]hept-2-ene, 2,3-diazabicyclo[2.2.2]oct-2-ene and their fused ring derivatives,<sup>163</sup> the molecular structures of the 1,3-diethoxycalix[4]crown-5-ether in the various isomers and their potassium-ion complexes,<sup>164</sup> *p*-*tert*-butylcalix[5]crown-6-ether complexed with alkylammonium ions,<sup>165</sup> the R- and Z-substituent effects for the gas-phase thermal decompositions of carbamates,<sup>166</sup> the sulfur dioxide absorption by organic Lewis bases,<sup>167</sup> the stable conformations of *p*-*tert*-butylcalix[4]arene crown ether bridged at the lower rim with pyridyl unit complexed with potassium ion,<sup>168</sup> and the potential energy functions for excited intramolecular proton transfer of salicylic acid and its derivatives.<sup>169</sup>

Some semiempirical calculations of structures are reported. See Refs. 145, 170, 171, 172, and 173.

Various theoretical techniques are used to determine structure-related quantities as well as structure themselves. The fragment reassociation method is used to determine Coulson, Mulliken and natural population analyses of several large molecules.<sup>174</sup> The structure, quantum mechanical force field and vibrational spectra of triphenylene are theoretically investigated.<sup>175</sup> The quantitative structure activity relationship is probed for mutagen X and spiro-succinimide-fused tetrahydropyrrolo[1,2-a]pyrazine-1,3-dione derivatives.<sup>176-178</sup> The monopole-macrodipole interactions in  $\alpha$ -helices are studied.<sup>179</sup> The s-bond activation of organic molecules by transition metal complexes are reviewed.<sup>180</sup> One-color nonlinear wavepacket interferometry signal calculations for a system of two electronic levels and one vibrational degree of freedom are presented.<sup>181</sup> First hyperpolarizabilities of nonlinear optical compounds are calculated.<sup>182</sup> The neural network studies are utilized to predict impact sensitivities of various types of explosive molecules.<sup>183</sup> Theoretical studies on predicting detonating

power of CHNO explosives are also reported.<sup>184</sup>

Structures of various molecules or complexes are determined experimentally. For example, new quaternary compounds ANb<sub>2</sub>PS<sub>10</sub> (A=Na, Ag) and AuNb<sub>4</sub>P<sub>2</sub>S<sub>20</sub> are synthesized and characterized.<sup>185</sup> The crystal structure of a new silver(I) dimer with isonicotinic acid is studied.<sup>186</sup> Fragmentations and ion-molecule reactions of ionized cyclohexane propionic acid and cyclohexane butyric acid are studied by using FTMS and theoretical calculations.<sup>187</sup> Molecular recognition for a specific cation depending on the change of the oxidation state of the metal catalyst component contained in the hydrogel network is studied in a self-oscillating hydrogel.<sup>188</sup> The [(Cu<sup>2+</sup>, Ni<sup>2+</sup>...Gly-Gly-His)-3H<sup>+</sup>]<sup>-1</sup> complex in gas phase is investigated by using the electrospray ionization mass spectroscopy.<sup>189</sup>

The methodologies used in quantum mechanical or thermodynamical calculations of molecular structure are either reviewed or suggested. The four-component and two-component relativistic molecular theories are surveyed.<sup>190</sup> Recent advances in multireference-based perturbation theory are reviewed.<sup>191</sup> *Ab initio* molecular dynamics with Born-Oppenheimer and extended Lagrangian methods is explained.<sup>192</sup> A thermodynamic perturbation method to calculate surface forces in confined-fluid systems is introduced.<sup>193</sup> Fundamental ideas of the free energy gradient method for determining transition structures are briefly reviewed.<sup>194</sup> Computational packages used in structure calculations are introduced, for example, recent development of linear scaling quantum theories in GAMESS,<sup>195</sup> ONIOM and its applications to material chemistry and catalyses,<sup>196</sup> and the three-dimensional molecular visualization and analysis program POSMOL.<sup>197</sup> Other methodology researches are the usage of rotation matrices in molecular dynamics simulations,<sup>198</sup> Gaussian-type basis sets on alkali metal iodides,<sup>199</sup> and construction of semi-diabatic potential energy surfaces of excited states by the equation-of-motion coupled-cluster method.<sup>200</sup>

Some pure theory related researches are reported. Rabi formula between the states of a coupled harmonic oscillator which may be used as a simple model for the electron transfer is derived.<sup>201</sup> The closed loop optimal control experiments are manipulated efficiently to steer the dynamics to lie within a subspace of the system eigenstates without requiring any prior detailed knowledge about the system Hamiltonian.<sup>202</sup> Spin and pseudo spins in theoretical chemistry are discussed.<sup>203</sup> The finite field method for calculating the fifth-order Raman response is developed.<sup>204</sup> Some new topological indices based on the distance matrix and Randic connectivity are proposed.<sup>205</sup> Canonical transformations for time-dependent harmonic oscillators are discussed.<sup>206</sup> Phase shifts of bound state waves scattered at classical turning points are studied.<sup>207</sup> Transition probabilities at crossing in the Landau-Zener problem are explained.<sup>208</sup> Supersymmetry for rigid symmetric top rotor is observed.<sup>209</sup> A theory for stimulated absorption and emission of photons between energy levels from the standpoint of discrete quantum jumps is presented.<sup>210</sup> The analytical transfer matrix method is

combined with supersymmetry to calculate the eigenenergies of Coulomb potential.<sup>211</sup> Artificial neural networks are successfully developed for the modeling and prediction of normalized polarity parameter of various solvents.<sup>212</sup>

**Macromolecules, Soft matter:** The fabrication and micropatterning of a hybrid composite like amorphous calcium carbonate and poly(ethylenimine) are reported.<sup>213</sup> Using spectroscopic techniques such as UV-VIS, IR, Raman, or NMR, crystals or molecular aggregates (for example, porphyrin-phthalocyanine aggregate, melaminium acetate acetic acid solvate monohydrate, and tetragonal  $\text{Cs}^+(15\text{-crown-5})_2\Gamma^-$ ) are characterized.<sup>214-216</sup> The syntheses and crystal structures of zeolite A, X, or Y are reported. The structure of molecules, clusters, or ions (for example,  $\text{PbI}_2$ ,  $\text{ZnI}_2$ ,  $\text{Ag}_4\text{Br}_4$ ,  $\text{K}^+$ ,  $\text{Cs}^+$ , and  $\text{TI}^+$ ) exchanged in the zeolite cavities are also investigated by using X-ray crystallography.<sup>217-222</sup>

Besides the crystallographic researches, the nanoporous film of  $\text{TiO}_2$  and  $\text{ZrO}_2$  and dibromobenzophenone choleic acid crystal are synthesized and their electronic properties are investigated.<sup>223,224</sup>

**Surfactants, Membranes:** There are few researches published in this topic, but a diversity in research may be found. The optimum conditions for the most effective precipitate of surfactant complex of sodium alkylsulfate with cetylpyridinium chloride are sought in aqueous solution.<sup>225</sup> Using two-dimensional correlation spectroscopy, thermal behavior of Langmuir-Blodgett film of poly(*tert*-butyl methacrylate) is studied.<sup>226</sup> Using reverse micellar systems, micelle-micelle interactions are studied.<sup>227</sup> The composite charged mosaic membrane endurance against mechanical pressure is investigated from the aspect of solute and solvent transport.<sup>228</sup>

**Statistical mechanics, Thermodynamics, Medium effects:** Based on statistical mechanics or thermodynamics, theories explaining some aspects of chemical reactions are suggested. The nonequilibrium distribution function theory is applicable to the relaxation kinetics of reversible reactions of the type  $\text{A}+\text{B} \leftrightarrow \text{C}+\text{B}$ .<sup>229</sup> The Wilemski-Fixman closure approximation and memory equations are suggested for diffusion-controlled or diffusion-influenced reactions.<sup>230,231</sup> The interaction potential switching effects in a reversible excited-state proton transfer reaction are investigated.<sup>232</sup> Noise effect in oscillating reaction model is studied.<sup>233</sup> The fractional diffusion equation is suggested for the anomalous diffusion on fractal lattices.<sup>234</sup> A direct and efficient method for estimating the entropy is suggested.<sup>235</sup> Anomalies of water in thin liquid films and in biological systems,<sup>236</sup> and the critical phase changes of a forward-scattered light in a nonpolar binary liquid mixture are studied.<sup>237</sup>

Thermodynamic properties of liquids and solutions are calculated. Free energy of Lennard-Jones fluids and square-well fluids, solvation free energy of the proton in methanol, acidity constants of benzoic acids and phenols in water, and the transfer enthalpy of urea from water to aqueous ethanol are calculated.<sup>238-241</sup> Dielectric analysis is performed for the H-bonded binary polar mixture in non-polar solvent.<sup>242</sup>

Molecular dynamics simulation or Monte Carlo simulation is used to determine chemical properties of various systems, for example, viscosity and diffusion constants of alkanes, spontaneous formation in the 1,4-cyclohexanedione-bromate-ferroin reaction, shear viscosity of benzene, toluene, and *p*-xylene, ionic mobility of  $\text{OH}^-$ , solvent effect on selectivity of 18-crown-6 to between  $\text{La}^{3+}$ ,  $\text{Nd}^{3+}$  and  $\text{Eu}^{3+}$  ion, and trap effects on the formation of space-charge field associated with the photorefractivity of nonlinear optical polymers.<sup>243-248</sup> Transport properties of various systems, *e.g.*, dumbbell molecules, liquid Ar, Ar-Kr mixtures, and diatomic liquids, are also calculated by dynamics simulation.<sup>249-252</sup> Dissipative particle dynamics simulation of bead-spring dumbbell models also appears.<sup>253</sup> There is one article which suggests a sampling method in simulation technique. It is the canonical sampling method for initial conditions for reactive flux calculations using Nose-Hoover chains.<sup>254</sup>

Physical chemistry in a medium is frequently studied. Solvent effects on rate constant of cycloaddition reaction of diethyl azodicarboxylate with ethyl vinyl ether are studied.<sup>255</sup> The complex solvent and the temperature dependence of the NMR shifts for the N- $\text{CH}_2$  protons in tris(*N,N*-diethyldithiocarbamate) iron(III) in various solvents are investigated to measure the effect of the solvent system on the environment of the transition metal ion.<sup>256</sup> Concentration and pH dependence of  $\beta$ -amyloid peptide conformations is studied.<sup>257</sup> The temperature dependence of *n*-octanol/water partition coefficients for sulfonamides is investigated.<sup>258</sup>

There are many theoretical researches on the systems related to a medium. For example, *ab initio* molecular orbital calculations on ion-pair interactions, in order to understand the effect of solvent induced inter-atomic attractions in various dielectric environments, are performed.<sup>259</sup> Using the solvation free energy density model, hydrophobicity of amino acids is calculated.<sup>260</sup> The applicability of the combined nearly ideal binary solvent/Redlich-Kister equation for correlation of various solvatochromic parameters with composition is searched.<sup>261</sup> A new method to reproduce the enthalpies of transfer of NaI from water to aqueous methanol, ethanol and PrOH solvent systems is suggested.<sup>262</sup> Partial molar heat capacity at infinite dilution for aqueous solutions of various polar aromatic compounds is studied by using artificial neural networks.<sup>263</sup>

**Biophysical chemistry:** Quantitative structure-activity relationship studies are frequently performed. The systems of interest are indolinones derivatives (as a potential inhibitor of the protein tyrosine kinase of fibroblast growth factor receptor), mutagen X and its analogs, angiotensin-converting enzyme inhibitors, microsomal prostaglandin  $\text{E}_2$  synthase inhibitors, and 6-nitroquipazine analogues as serotonin transporter.<sup>264-269</sup>

Theoretical modeling studies (for example, *ab initio* calculation, dynamics simulation, molecular docking, homology-based modeling) reveal various biophysical informations. They are homodimerization of thalictrum tuberosum *o*-methyltransferases, the binding free energy of four different protonated states of HIV-1 protease with inhibitor, a

structure of alpha-helix motif, the inhibition mechanism of natural ligands to farnesyl protein transferase, the solution structures of four *diploptera punctata* allostatins, and the binding modes of cationic *meso*-tetrakis(*N*-methylpyridinium-4-yl)porphyrin to d[(GCATATATGC)<sub>2</sub>] duplex.<sup>270-274</sup>

Experimentally, using spectroscopy, microscopy, and X-ray scattering, biophysical systems are investigated. The solution structures of four *diploptera punctata* allostatins are determined by using NMR spectroscopy.<sup>273</sup> Amyloid aggregates are imaged by using fluorescence lifetime imaging microscopy.<sup>275</sup> Binding of norfloxacin to wide variety of DNA, DNA mediated energy transfer from 4',6-diamidino-2-phenylindole to Ru(II)[(1,10-phenanthroline)<sub>2</sub>L]<sup>2+</sup>, and binding of naringenin derivatives and cyclin dependent kinase are all spectroscopically studied.<sup>276-278</sup> The doxorubicin binding sites and the structural variations of doxorubicin-DNA complexes in an aqueous solution are determined by using UV-resonance Raman spectroscopy and surface enhanced Raman spectroscopy.<sup>279</sup> Fine structures of photoactive yellow protein in solution are explored by using wide-angle X-ray scattering.<sup>280</sup> By monitoring the variance of fluorescence intensity the denaturation of guanidine is observed.<sup>281</sup>

Conformational dynamics studies are also performed. The conformational dynamics of heme pocket, a small vacant site near the binding site of heme proteins-myoglobin and hemoglobin, is investigated by using the time-resolved vibrational spectroscopy.<sup>282-284</sup> In addition, excitability which is one of the basic and fundamental mechanisms utilized for signal transmission in living organisms is studied.<sup>285</sup> The technique of nanoliter reactor arrays that can be used for discovery of drugs is applied to monitoring how the antibiotic gramicidin embedded lipid vesicles functions by dispensing acidic drops.<sup>286</sup>

**Nanoparticles and nanostructures:** Since many of nanochemistry related researches are submitted to the material chemistry associate editor, there appear to be few PC articles on this topic in BKCS. A novel tool for studying in-situ dynamics of nanoparticles, *i.e.*, single nanoparticle ion trap, is introduced.<sup>287</sup> Using the tip-induced quenching technique high-resolution fluorescence image of individual nanoparticles is obtained.<sup>288</sup> Theoretical calculations reveal that the fine-structures of nanoparticles at gold nanosphere-gold plane junctions play a significant role in SERS activity.<sup>289</sup> Laser desorption and ionization of vertically aligned carbon nanotube arrays are reported.<sup>290</sup> Chemistry of nanoparticles on substrates is also investigated. They are plasmon resonance of Ag nanoparticles on highly ordered pyrolytic graphite, Au nanoparticles at the liquid/liquid interface, Pd nanoparticles and gold nanoplates at the water/oil interface, and Au nanoparticles-embedded plasticized polymer membrane.<sup>291-295</sup> Fabrication and characterization of nanoparticles are also pursued, for example, CdS/Ag metal-semiconductor composite quantum dots and PMMA-coated CdS nanorod.<sup>296,297</sup>

**Surfaces, Interfaces, Catalysis:** The nature of surface is studied, *i.e.*, the secondary electron yield is measured from the high-energy proton bombardment on Al target.<sup>298</sup> The

behavior of hydrogen-terminated Si(111) surface in oxygen-dissolved NH<sub>4</sub>F solution is studied.<sup>299</sup> The character of species adsorbed on surface is frequently investigated. The adsorptions and configurations of CO on W(110) and W(100) surfaces are studied by molecular orbital theory.<sup>300</sup> The structure of ethephone adsorbed on silver surface is investigated by SERS.<sup>301</sup> Benzene on Si surface is imaged and manipulated by using a variable-low temperature scanning tunneling microscope.<sup>302</sup> Self-assembled monolayers of aromatic thiol on Au(111), cyclopentanethiol on Au(111), mercaptoacetic acid on Ag, azobenzene-incorporated alkanethiol on silver, and single 3C-SiC thin films on Si(100) are characterized.<sup>303-307</sup> As for interface researches, phosphatidylcholine monolayers with different alkyl chains at the air/water interface are investigated.<sup>308</sup>

Surface mediated reactions are also frequently studied. They are the substrate dependency of surface-induced photo-reaction of organic monolayers on silver, the surface chemistry of ammonium hydroxide with Zircaloy-4, and cleavage of disulfide bond during the self-assembly processes of unsymmetric dialkyl disulfides on Au(111).<sup>309-311</sup> More examples are the interaction of SO<sub>2</sub> with oxygen on Ni(100), reactions of NO on a VO/V(110) surface, the reaction of Ar-ion with D<sub>2</sub>O dosed Zircaloy-4 surface, and the annealing effect of tolanethioacetate self-assembled monolayers on Au(111).<sup>312-315</sup>

Reactions on surface are investigated theoretically, for example, formation of hydroxyl radical from the hydrogen chemisorbed silicon surface by incident oxygen atoms, formation of HBr between gas-phase bromine atom and chemisorbed hydrogen atoms on a Si(001) surface, reaction between gas-phase hydrogen atom and chemisorbed bromine atoms on a Si(001) surface, and the formation and hydrogenation of carbon for CO<sub>2</sub> methanation on the Ni(111) surface.<sup>316-319</sup> The photodesorption of Xe from an oxidized Si(001) surface is also theoretically studied.<sup>320</sup>

Researches related to catalysis are reported. Catalytic activities of perovskite-type LaBO<sub>3</sub> (B = Fe, Co, Ni) oxides for partial oxidation of methane are investigated.<sup>321</sup> The role of bifunctional catalysts in hydrolysis reactions of *N*-benzoyl-4(5)-methylimidazoles is reported.<sup>322</sup> The character of calcium oxide catalysts for activation of methane to C<sub>2</sub> hydrocarbons and the nanometer-sized TiO<sub>2</sub>, V-TiO<sub>2</sub>, and Pt/V-TiO<sub>2</sub> photocatalysts for photodecomposition of concentrated ammonia are investigated.<sup>323,324</sup> The catalytic activities of nickel-based catalysts are estimated for oxidizing acetaldehyde of volatile organic compounds.<sup>325</sup>

**Electron transport, Optical and electronic devices:** On this topic, there are few articles published in BKCS. But related researches can be found. In Ref. 326, the structures of polyheterocyclic derivatives with vinylenediheteroatom substituents are quantum mechanically studied. These compounds can be used in blue-light-emitting devices. In Ref. 327, the structures of polypentafulvalenes, which are environmentally stable semiconductive or conductive polymers, are investigated. A new material, *e.g.*, indium-doped zinc oxide thin film that can be used in organic light emitting devices, is

**Table 2.** Number of all articles and PC articles published in BKCS and JACS

Journal	Year	All articles	PC articles (%)
BKCS	2003	411	90(22%)
	2004	430	65(15%)
	2005	432	61(14%)
	2006	421	57(14%)
	2007	499	73(15%)
	Total	2193	346(16%)
JACS	2007	2957	336(11%)

suggested.<sup>328</sup>

**Energy conversion and storage:** On this topic, there are no articles published in BKCS.

### BKCS Compared with JACS and JPC

The comparison analysis is performed with the articles published in BKCS from 2003 through 2007 and the articles in JACS of 2007. Since the analysis is focused on the ratio (or percentage) of articles under consideration, the absolute number of articles included in the study may not be meaningful. However, the number of PC articles published in BKCS each year is so small that the recent 5 year articles of BKCS are chosen for comparison.

The BKCS and JACS are multidisciplinary chemistry journals both publishing research works in all branches of chemistry. As shown in Table 2, BKCS publishes 400-500 articles a year, and the total of 2193 articles are published from 2003 to 2007. Among them, the authors find the 346 articles as the PC articles. A content analysis to decide whether it is a PC article or not is performed; the authors examined each article. The proportion of physical chemistry researches (=the number of PC articles divided by the number of all articles) in BKCS is 16% ( $= 346/2193 \times 100$ ) in average for the last 5 years. JACS published 2957 articles in 2007 and the 336 articles are found to be PC articles. Thus

**Table 3.** Nationality of authorship of PC articles published in BKCS and JACS

Journal	Year	Number of PC articles	
		Korean	Non-Korean
BKCS	2003	71(79%)	19(21%)
	2004	60(92%)	5(8%)
	2005	54(89%)	7(11%)
	2006	50(88%)	7(12%)
	2007	68(93%)	5(7%)
	Total	303(88%)	43(12%)
JACS	2007	US	Non-US
		160(48%)	176(52%)

the physical chemistry proportion of JACS is 11% ( $= 336/2957 \times 100$ ). The PC proportions of BKCS and JACS are found to be similar. Considering that JACS is a high impact chemistry journal and probably the most prestigious and widely read chemistry journal in the world,<sup>329-331</sup> it is encouraging that BKCS represents physical chemistry researches as much as JACS does.

Non-Korean researchers publish 12% of PC articles in BKCS, whereas 52% of PC articles published in JACS are authored by non-US researchers. (See Table 3 for the details.) The foreign authorship ratio of BKCS (*i.e.*, the number of non-Korean author PC articles divided by the number of all PC articles  $= 43/346 \times 100 = 12\%$ ) is very low compared with the foreign authorship ratio of JACS (*i.e.*, the number of non-US author PC articles divided by the number of all PC articles  $= 176/336 \times 100 = 52\%$ ). One of the reasons for JACS's prestige may come from participation by a large number of chemists worldwide. To be a world leading journal, the BKCS should solicit submissions from abroad more extensively.

An in-depth content analysis is performed for the BKCS PC articles to decide a topic where a particular article belongs. The 12 topic classification used in JPC is utilized in this analysis to make a comparison between BKCS and JPC.

**Table 4.** Number of PC articles published in BKCS and JPC in 12 topics

Topics	BKCS (2003-2007)	JPC (2007)
Dynamics/Clusters/Excited states	34(10%)	299(5%)
Kinetics/Spectroscopy	82(24%)	500(8%)
Atmospheric, environmental and green chemistry	0(0%)	97(2%)
Molecular structure/Quantum chemistry/General theory	108(31%)	746(12%)
Macromolecules/Soft matter	13(4%)	523(8%)
Surfactants/Membranes	5(1%)	250(4%)
Statistical mechanics/Thermodynamics/Medium effects	38(11%)	502(8%)
Biophysical chemistry	23(7%)	558(9%)
Nanoparticles and nanostructures	11(3%)	1030(17%)
Surfaces/Interfaces/Catalysis	29(8%)	1267(21%)
Electron transport/Optical and electronic devices	3(1%)	259(4%)
Energy conversion and storage	0(0%)	136(2%)
Total	346(100%)	6167(100%)

JPC is chosen as a reference journal because it is a premier physical chemistry journal that reflects the physical chemistry researches worldwide. JPC A, B, and C, each covering four topics, published 6167 articles altogether in 2007. JPC A publishes physical chemistry articles in "Dynamics, Clusters, Excited states", "Kinetics, Spectroscopy", "Atmospheric, environmental and green chemistry", and "Molecular structure, Quantum chemistry, General theory". JPC B publishes articles in "Macromolecules, Soft matter", "Surfactants, Membranes", "Statistical mechanics, Thermodynamics, Medium effects", and "Biophysical chemistry". Four topics covered in JPC C are "Nanoparticles and nanostructures", "Surfaces, Interfaces, Catalysis", "Electron transport, Optical and electronic devices", and "Energy conversion and storage".

The results of classification of the BKCS PC articles into 12 topics are summarized in Table 4. It lists the number of PC articles in each topic for BKCS and JPC. The number of articles published in JPC in the following four topics, *i.e.*, "Atmospheric, environmental and green chemistry ( $2\% = 97/6167 \times 100$ )", "Energy conversion and storage ( $2\% = 136/6167 \times 100$ )", "Surfactants, Membranes ( $4\% = 250/6167 \times 100$ )", or "Electron transport, Optical and electronic devices ( $4\% = 259/6167 \times 100$ )", is less than or equal to 4% of the number of all articles published. In BKCS, the number of PC articles in the same four topics is almost nil. The four topics are not well represented in both JPC and BKCS probably because there are many other journals that cover those topics.

The most frequently published topics in JPC are "Surfaces, Interfaces, Catalysis ( $21\% = 1267/6167 \times 100$ )", "Nanoparticles and nanostructures ( $17\% = 1030/6167 \times 100$ )", and "Molecular structure, Quantum chemistry, General theory ( $12\% = 746/6167 \times 100$ )". While in BKCS, they are "Molecular structure, Quantum chemistry, General theory ( $31\% = 108/346 \times 100$ )", "Kinetics, Spectroscopy ( $24\% = 82/346 \times 100$ )", and "Statistical mechanics, Thermodynamics, Medium effects ( $11\% = 38/346 \times 100$ )". Hot topics such as surface chemistry and nano-chemistry are well represented in JPC, but traditional topics such as molecular structure and spectroscopy are well represented in BKCS. It does not mean that surface chemistry or nano-chemistry is not widely researched by the BKCS authors. Rather it indicates that BKCS does not absorb the surface or nano-chemistry researches adequately. Nonetheless, all major topics of physical chemistry are covered in BKCS.

As shown in Table 3, 88% of the PC articles published in BKCS are authored by Koreans. Therefore one may conclude that the analyses conducted in this work on BKCS PC articles is representing the research interest of Korean physical chemists in general. However, the authors of this work advise that the results of this study should be viewed cautiously, because a major portion of research performed by Korean researchers are published in journals other than BKCS. In 2006, Koreans published the 386 PC articles in SCI journals.<sup>332</sup> In the same year, 50 PC articles having a Korean authorship were published in BKCS which is one of SCI journals. That is, the BKCS absorbs only 13% of all PC

articles published by Koreans. It is to be noted for reference purpose that the number of Korean-author PC articles published in 2007 in JACS and JPC are 7 (or  $2\% = 7/336 \times 100$ ) and 126 (or  $2\% = 126/6167 \times 100$ ), respectively.

### Concluding Remarks

The contents of the PC articles in BKCS are summarized in this work, and it clearly reveals that the current trend of the physical chemistry researches are represented adequately in BKCS. It is found that the physical chemistry research topics covered in the journal are diverse though some topics such as surface chemistry or nano-chemistry are under-represented.

Suggestions for BKCS to be a world leading journal are as follows. BKCS should increase the number of articles extensively although it may not reach up to the level comparable to JACS which is also a multidisciplinary chemistry journal. Then the number of PC articles will naturally increase to a degree for which a separate section for physical chemistry articles can be formulated within the journal. It is necessary because there is no 'physical chemistry journal' published in Korea currently. BKCS must solicit more contributions from non-Korean nationals. In order to solicit more articles internationally, the visibility of BKCS should be greatly improved. One way of making this possible is to provide a means for easy public access to BKCS. It is urgent and absolutely necessary to make the current on-line database of BKCS (*i.e.*, electronic journal of BKCS) linked to the worldwide information network and open for barrier-free access. Recently the SCI impact factors (a commonly acknowledged index of a journal quality) of BKCS are steadily increasing: 0.706 (year 2003), 0.890 (2004), 0.918 (2005), and 0.950 (2006). It is expected that all these efforts will work together to make BKCS more visible internationally, and in turn it will attract more research papers with quality which will increase the citations, and thus the impact factor of BKCS.

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332. Since the bibliographic data of SCI journals for the year of 2007 are not yet complete at the time of writing this work (as of January 1st 2008), the data for 2006 are taken as a reference. Using the SCI-Expanded database with the search condition of "Py = 2006; Cu = South Korea; DocType = Article, Review, Letter; Language = All languages; Database = SCI-EXPANDED; Timespan = 1995-2008", all the SCI journals containing at least one Korean authorship article are selected. Then, 89 journals that may contain PC articles are hand picked. Again using the SCI-Expanded database with the search condition of "Source = BULLETIN OF THE KOREAN CHEMICAL SOCIETY, THIN SOLID FILMS, ... (the 89 source titles)", 1983 articles are selected. Finally analyzing the contents of the articles one by one, the authors obtain 386 PC articles by Koreans published in SCI journals in 2006.