Included in this print edition:
Issue 1 (January 5, 2015)
Issue 2 (January 15, 2015)

Journal of COMPUTATIONAL CHEMISTRY

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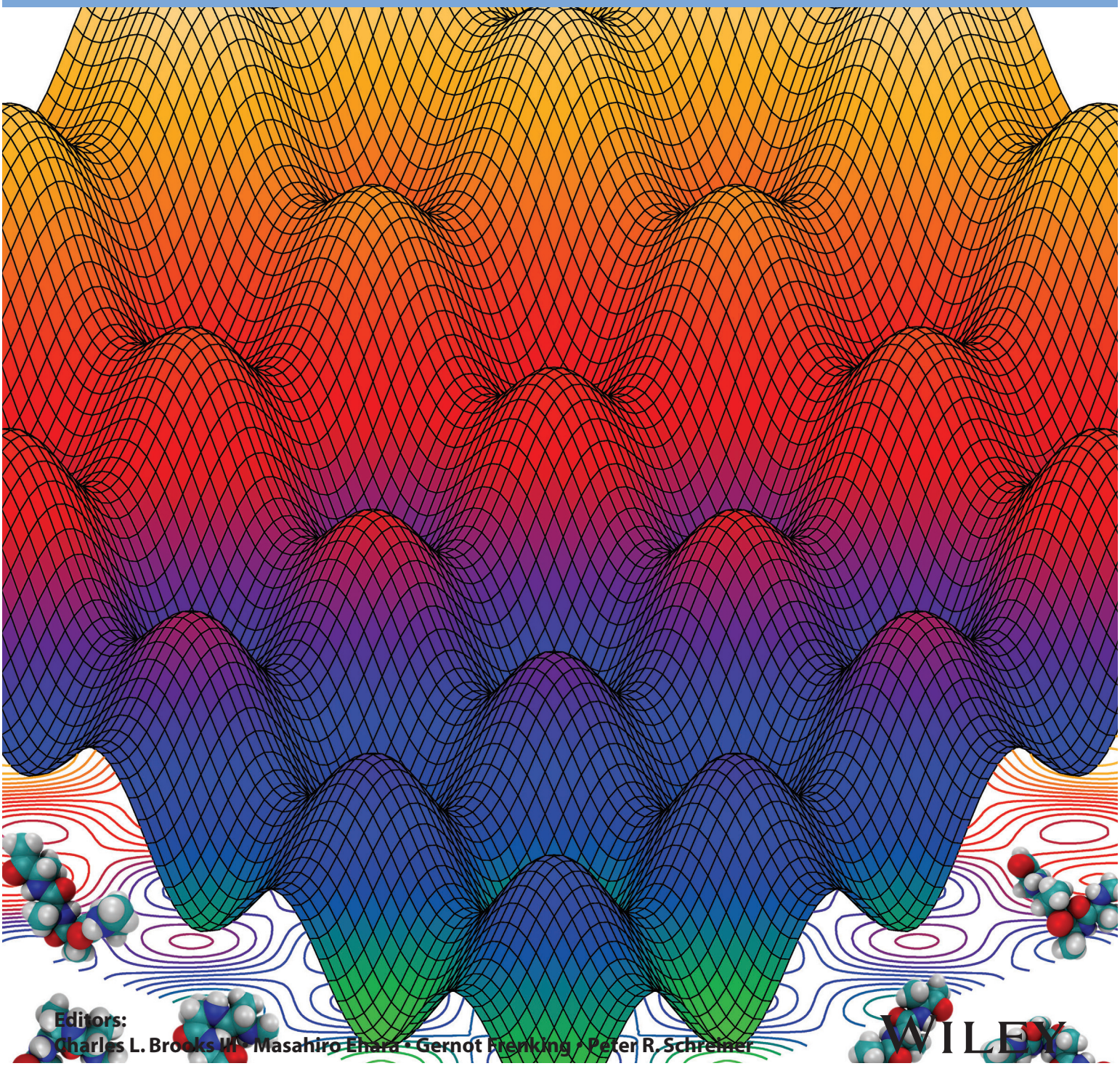

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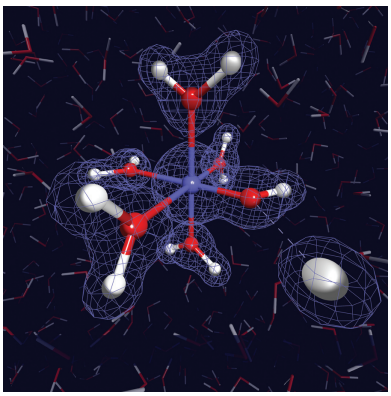
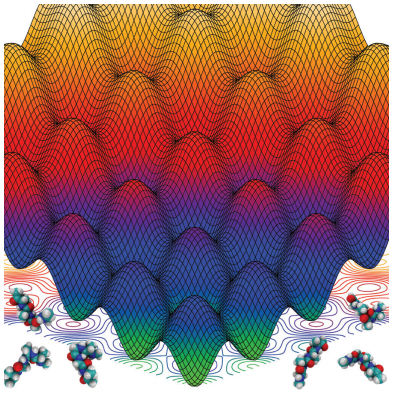


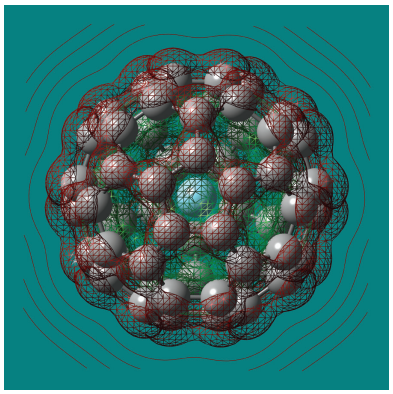
Hexa-Aqua Transition Metal Complexes

Aqueous pK_A values for hexa-aqua complexes of first and second row transition metals are computed using a combination of quantum chemical and electrostatic methods. On page 69, Gegham Galstyan and Ernst-Walter Knapp report the computed pK_A values show very good agreement with measured pK_A values with a root mean square deviation of 1 pH unit. Compared to previous approaches, the precision of the method is systematically improved.



Molecular Dynamics

On page 79, Robin M. Betz and Ross C. Walker report on Paramfit, a new program that generates force field parameters for molecular dynamics simulation by minimizing the difference between *ab-initio* quantum and classical energies of a set of input molecular conformations. The program incorporates a novel minimization algorithm capable of reliably locating global minima, shown by testing on various surfaces like the three-dimensional Rastrigin function illustrated here, which features numerous attractive local minima. Several molecular conformations of a small peptide used for demonstrating the program's efficacy on biological systems are also shown at the border. Structures like these are input into Paramfit, along with associated quantum energies, and are used to generate parameters of interest.



Rare Gas Encapsulation

Encapsulating rare-gas atoms into fullerenes smaller than C_{60} quickly becomes repulsive and follows an exponential law with decreasing number of carbon atoms. The reason comes from a rather rigid cage structure that determines the space available inside the fullerene. On page 88, Rebecca Sure, Ralf Tonner, and Peter Schwerdtfeger provide detailed insight into rare-gas fullerene interactions ranging from C_{20} to C_{60} and from He to Ar using Grimme's dispersion corrected density functional theory. The maximum inscribing inner sphere inside a fullerene cage gives a good qualitative picture for the space available.

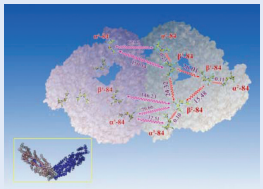
Coming Soon

Look for these important papers in upcoming issues

Clarifying and illustrating the electronic energy transfer pathways in trimeric and hexameric aggregation state of cyanobacteria allophycocyanin within the framework of Förster theory

Yanliang Ren et al.

The electronic energy transfer is a fundamental key in the development of synthetic light-harvesting devices. Insight into the EET pathways in cyanobacteria allophycocyanin trimer and hexamer is gained by the first principle calculations within the framework of Förster theory.
DOI: 10.1002/jcc.23770



Isolated pentagon rule violating endohedral metallofullerenes explained using the Hückel rule: A statistical mechanical study of the c_{84} isomeric set

Timothy Fuhrer et al.

A systematic, temperature dependent, statistical thermodynamic study is presented of the 24 possible isolated pentagon rule fullerene isomers of C_{84} as well as two of the experimentally known non-IPR isomers (51365 and 51383), at several different charges (0, −2, −4, and −6). Based on the results, the Hückel rule is a valid explanation for the stability of fused pentagons in endohedral metallofullerenes.
DOI: 10.1002/jcc.23774