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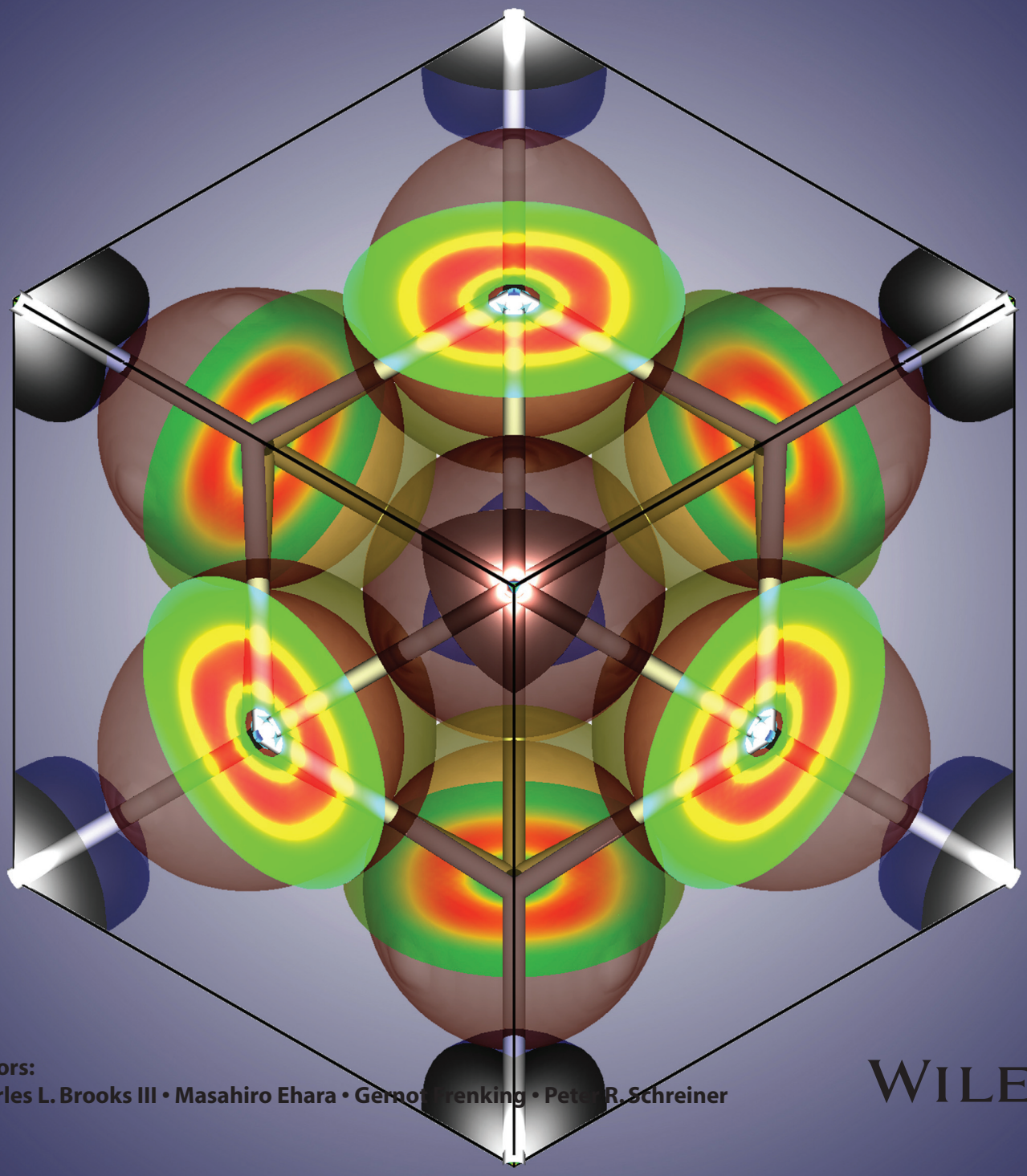

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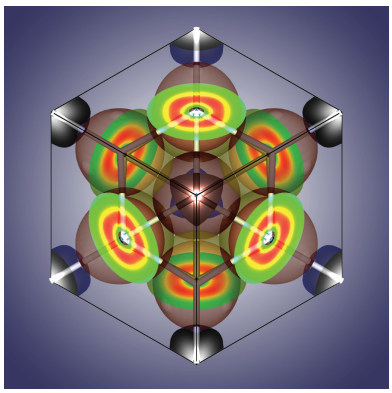
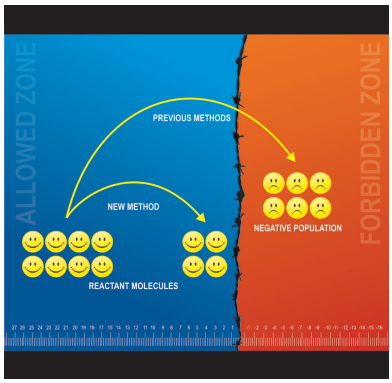


Extending Hirshfeld-I

The image shows an isosurface of Hirshfeld-I "atoms in molecules" for Ti-doped CeO_2, taken at an electron density of 0.03e/A^3, as presented by Danny E. P. Vanpoucke, Patrick Bultinck, and Isabel Van Driessche on page 405. The cubic $Ce_{0.75}Ti_{0.25}O_2$ unit cell is shown along the 111 direction. The different atoms are still clearly distinguishable at this iso-surface level, and show the Ti atom in the corners to be much smaller than the Ce atoms on the sides. In this issue, this implementation of the Hirshfeld-I method for solids is published back to back with a Comment from Thomas A. Manz and the authors' Reply.



Accelerated Stochastic Simulations

Many approximate accelerated stochastic simulation methods exist that can provide a means of employing Kinetic Monte Carlo techniques to model chemical kinetics. The drawback in using such methods is that sometimes the population of the reactant species present during the simulations becomes negative, leading to unphysical results. This is due to the manner in which the change in time during the reactions is handled by the stochastic simulation methods in such systems. The work by Shantanu Kadam and Kumar Vanka on page 394 discusses a means of avoiding this problem by combining the representative reaction approach (RRA) based methodology with the stochastic simulation algorithm (SSA) and the binomial method.

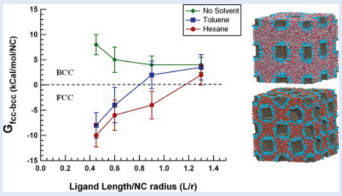
Coming Soon

Look for these important papers in upcoming issues

Solvent-driven symmetry of self-assembled nanocrystal superlattices—A computational study

Ananth P. Kaushik and Paulette Clancy

The preference of facetted Pb chalcogenide nanocrystals to spontaneously choose a crystal habit for superlattices is investigated. The thermodynamic stability of the superlattice and its preference of symmetry as the length of the ligand chains and the choice of solvent are varied are studied. The free energy difference between FCC and BCC superlattice symmetries is evaluated to determine the system's preference for either geometry. DOI: 10.1002/jcc.23152



$(Ala)_4$-X-$(Ala)_4$ as a model system for the optimization of the χ1 and χ2 amino acid side-chain dihedral empirical force field parameters

Jihyun Shim et al.

In this work, the $(Ala)_4$-X-$(Ala)_4$ peptide, were X is any amino acid, serves as model system that mimics the conformations of side-chains sampled in simulations of full proteins. Accordingly, $(Ala)_4$-X-$(Ala)_4$ represents a model system that will be of utility for the iterative parameterization of protein side-chain dihedral parameters. DOI: 10.1002/jcc.23178