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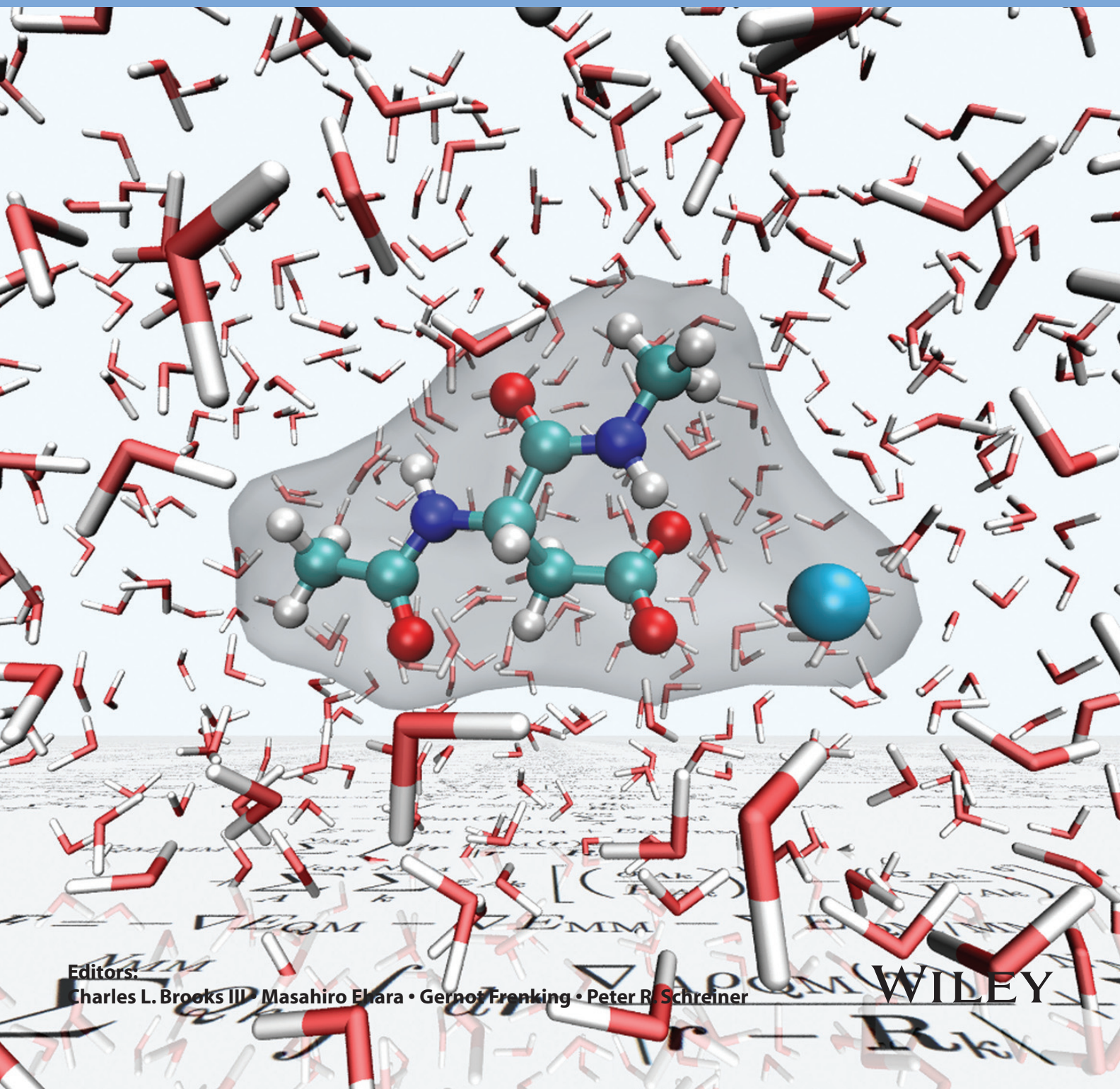

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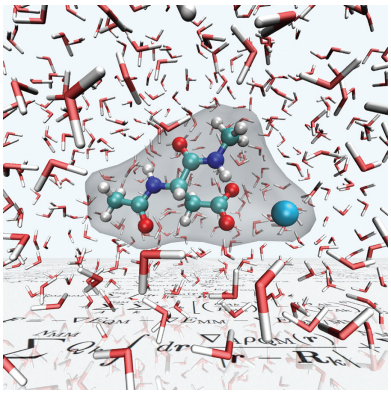
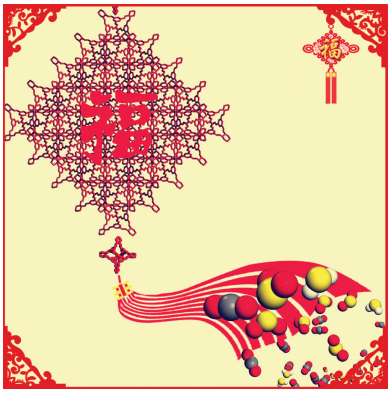


Calcium Binding

The cover shows a calcium ion coordinating to aspartate in aqueous solution, used by Andreas Götz, Matthew Clark, and Ross Walker on page 95 to demonstrate features of a new interface to electronic structure programs for *ab initio* wave function theory and DFT-based QM/MM simulations with the AMBER software package. Data exchange between the programs is implemented by means of files and system calls or the message passing interface. The QM/MM equations governing the implementation are visible on the surface that extends to the horizon.



Grand Canonical Monte Carlo

To accurately predict the adsorption of pollution gases (CO_2, SO_2, H_2S, and CO) in a porous organic cage CC3, Wenliang Li and Jingping Zhang propose a general multi-scale simulation procedure on page 174. In detail, the B2PLYP-D3/def2-TZVPP method is validated by CCSD(T)/CBS and then used to produce reference data for fitting an intermolecular force field *vdW3* that is subsequently used in grand canonical Monte Carlo (GCMC) simulations. There is good agreement of CO_2 uptake between GCMC simulation results and experimental data. The low deviation for SO_2, H_2S, and CO makes the approach suitable for predicting gases in novel porous materials.

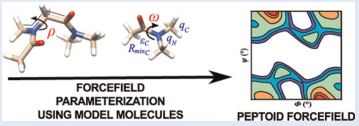
Coming Soon

Look for these important papers in upcoming issues

Development and use of an atomistic CHARMM-based force field for peptoid simulation

Dina T. Mirijanian et al.

Experiments and quantum mechanical calculations are used to develop an atomistic CHARMM-based force field for peptoids, technologically important positional isomers of peptides.
DOI: 10.1002/jcc.23478



A polarizable dipole–dipole interaction model for evaluation of the interaction energies for N–H···O=C and C–H···O=C hydrogen-bonded complexes

Shu-Shi Li et al.

A polarizable dipole–dipole interaction model is established to estimate the equilibrium hydrogen bond distances and the interaction energies for hydrogen-bonded complexes containing peptide amides and nucleic acid bases. The magnitude of the bond dipole moment varies according to its environment.
DOI: 10.1002/jcc.23473