This Special Topic is dedicated to the ongoing efforts of the theoretical chemistry community to develop a new generation of accurate force fields based on data from high-level electronic structure calculations and to develop faster electronic structure methods for testing and designing force fields as well as for carrying out simulations. This collection includes a 36 original research articles that illustrate recent theoretical advances in the field. It provides a timely snapshot of recent developments in the generation of approaches to enable more accurate molecular simulations of processes important in chemistry, physics, biophysics, and materials science. You can read more about the Special Topic in the Preface by the Guest Editors. We hope you enjoy it!

With Guest Editors Ken Jordan and Jean-Philip Piquemal

Preface: Special Topic: From Quantum Mechanics to Force Fields

Jean-Philip Piquemal and Kenneth D. Jordan
DOI: 10.1063/1.5008887

The BioFragment Database (BFDb): An open-data platform for computational chemistry analysis of noncovalent interactions

DOI: 10.1063/1.5001028

Fast divide-and-conquer algorithm for evaluating polarization in classical force fields

Dominique Nocito and Gregory J. O. Beran
DOI: 10.1063/1.4977981

Cheap but accurate calculation of chemical reaction rate constants from ab initio data, via systemspecific, black-box force fields

Julien Steffen and Bernd Hartke
DOI: 10.1063/1.4979712

Electrostatic solvation free energies of charged hard spheres using molecular dynamics with density functional theory interactions

Timothy T. Duignan, Marcel D. Baer, Gregory K. Schenter, and Christopher J. Mundy
DOI: 10.1063/1.4994912

Mapping the Drude polarizable force field onto a multipole and induced dipole model

Jing Huang, Andrew C. Simmonett, Frank C. Pickard IV, Alexander D. MacKerell Jr, and Bernard R. Brooks
DOI: 10.1063/1.4984113
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<td>Analytical gradients for tensor hyper-contracted MP2 and SOS-MP2 on graphical processing units</td>
<td>J. Chem. Phys.</td>
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<td>Chenchen Song and Todd J. Martinez</td>
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<td>Minimal distributed charges: Multipolar quality at the cost of point charge electrostatics</td>
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<td>Oliver T. Urke, Mike Deveraux, and Markus Meuwly</td>
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<td>Organic ion association in aqueous phase and ab initio-based force fields: The case of carboxylate/ammonium salts</td>
<td>J. Chem. Phys.</td>
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<td>Céline Houriez, Valérie Vallet, Florent Réal, Michael Meot-Ner (Mautner), and Michel Masella</td>
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<td>A general intermolecular force field based on tight-binding quantum chemical calculations featured</td>
<td>J. Chem. Phys.</td>
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<td>Stefan Grimme, Christoph Bannwarth, Eike Caldeweyher, Jana Pisarek, and Andreas Hansen</td>
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<td>Assessing many-body contributions to intermolecular interactions of the AMOEBA force field using energy decomposition analysis of electronic structure calculations</td>
<td>J. Chem. Phys.</td>
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<td>Omar Demerdash, Yuezhi Mao, Tianyi Liu, Martin Head-Gordon, and Teresa Head-Gordon</td>
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<td>Performing the Millikan experiment at the molecular scale: Determination of atomic Millikan-Thomson charges by computationally measuring atomic forces</td>
<td>J. Chem. Phys.</td>
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<td>T. Ryan Rogers and Feng Wang</td>
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<td>Two-component, ab initio potential energy surface for CO₂—H₂O extension to the hydrate clathrate, CO₂ṣ(H₂O)₂₀, and VSCF/VCI vibrational analyses of both</td>
<td>J. Chem. Phys.</td>
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<td>161714</td>
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<td>Qingfeng (Kee) Wang and Joel M. Bowman</td>
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<td>Structure and polarization near the Li⁺ ion in ethylene and propylene carbonates</td>
<td>J. Chem. Phys.</td>
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<td>Travis P. Pollard and Thomas L. Beck</td>
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<td>Structural study of Na₂O–B₂O₃–SiO₂ glasses from molecular simulations using a polarizable force field</td>
<td>J. Chem. Phys.</td>
<td>147</td>
<td>161711</td>
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<td>Fabien Pacaud, Jean-Marc Delaye, Thibault Charpente, Laurent Cormier, and Mathieu Salanne</td>
<td>10.1063/14992799</td>
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## From dimers to the solid-state: Distributed intermolecular force-fields for pyridine


Alexander A. Aina, Alston J. Misquitta, and Sarah L. Price  
DOI: [10.1063/1.4999789](https://doi.org/10.1063/1.4999789)

## Development of reactive force fields using ab initio molecular dynamics simulation minimally biased to experimental data


Chen Chen, Christopher Arntsen, and Gregory A. Voth  
DOI: [10.1063/1.4985903](https://doi.org/10.1063/1.4985903)

## Combining configurational energies and forces for molecular force field optimization


Lukas Vlcek, Weiwei Sun, and Paul R. C. Kent  
DOI: [10.1063/1.4986079](https://doi.org/10.1063/1.4986079)

## Improving the accuracy of Møller-Plesset perturbation theory with neural networks


Robert T. McGibbon, Andrew G. Taube, Alexander G. Donchev, Karthik Siva, Felipe Hernández, Cory Hargus, Ka-Hei Law, John L. Klepeis, and David E. Shaw  
DOI: [10.1063/1.4986081](https://doi.org/10.1063/1.4986081)

## Understanding the many-body expansion for large systems. III. Critical role of four-body terms, counterpoise corrections, and cutoffs


Kuan-Yu Liu and John M. Herbert  
DOI: [10.1063/1.4986110](https://doi.org/10.1063/1.4986110)

## Quasi-chemical theory of F−(aq): The “no split occupancies rule” revisited


Mangesh I. Chaudhari, Susan B. Rempe, and Lawrence R. Pratt  
DOI: [10.1063/1.4986244](https://doi.org/10.1063/1.4986244)

## Implementation of analytical gradients and of a mixed real and momentum space DVR method for excess electron systems described by a self-consistent polarization model


Tae Hoon Choi, Tijo Vazhappilly, and Kenneth D. Jordan  
DOI: [10.1063/1.4990396](https://doi.org/10.1063/1.4990396)

## Building better water models using the shape of the charge distribution of a water molecule


Charnila Chathuranga Dharmawardhana and Toshiko Ichiye  
DOI: [10.1063/1.4986070](https://doi.org/10.1063/1.4986070)

## Computer simulations of alkali-acetate solutions: Accuracy of the forcefields in difference concentrations


Emma Ahlstrand, Julio Zukerman-Schpector, and Ran Friedman  
DOI: [10.1063/1.4985919](https://doi.org/10.1063/1.4985919)

## The truncated conjugate gradient (TCG), a non-iterative/fixed-cost strategy for computing polarization in molecular dynamics: Fast evaluation of analytical forces


Félix Aviat, Louis Lagardère, and Jean-Philip Piquemal  
DOI: [10.1063/1.4985911](https://doi.org/10.1063/1.4985911)

## Study of interactions between metal ions and protein model compounds by energy decomposition analyses and the AMOEBA force field


Zhifeng Jing, Rui Qi, Chengwen Liu, and Pengyu Ren  
DOI: [10.1063/1.4985921](https://doi.org/10.1063/1.4985921)