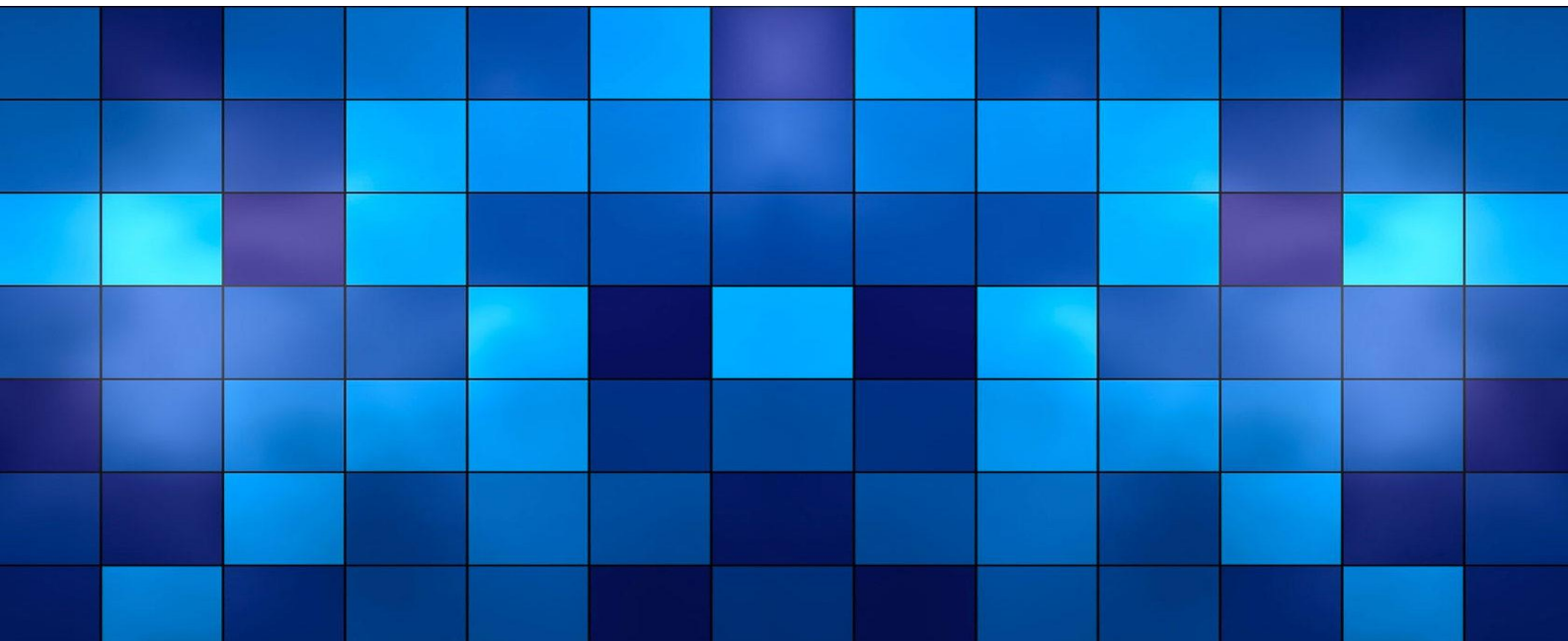


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 Xuechen Li, Suhuai Luo, and Qingmao Hu
 A rib locating method on chest direct radiography

At the bottom, there is a "Cloud Explorer" section with various scientific terms like "ab initio calculations", "adsorption", "aluminum", "annealing", "atomic force", "microscopy", "copper", "crystal structure", "density functional theory", "design", "diffusion", "electrochemical", "electrodes", "electrochemistry", "electronic structure", "elemental", "semiconductors", "energy gap", "etching", "excited".

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Argyris Kahros and Benjamin J. Schwartz
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(Received 16 June 2013; accepted 9 September 2013; published online 8 October 2013)



Abstract
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3

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Stoll, Fuentealba, and Szentpály (SFS) argue that the coordinate-dependent pseudopotential we developed for the sodium dimer cation molecule is inferior to other potentials that have been presented in the literature for this molecule. The goal of our work, however, was to present a novel method for the development of rigorous coordinate-dependent pseudopotentials. Our method is designed to reproduce all-electron Hartree-Fock calculations without the inclusion of adjustable parameters. Moreover, our method starts from the superposition of unoptimized, non-norm-conserved atomic potentials, so that when complete, the resulting norm-conserving potential can reproduce an all-electron Hartree-Fock calculation without the inclusion of adjustable parameters. We chose the sodium dimer cation system as a proof of principle for our method, and showed that our method does indeed allow a one-electron calculation to correctly reproduce the all-electron Hartree-Fock calculation from bonding to the dissociation limit. Our purpose in developing this method is to use such potentials in condensed-phase mixed quantum/classical molecular dynamics simulations, where inclusion of valence polarization effects is unimportant or can be added on after the fact. Thus we do not claim that our method provides a potential that is superior to potentials

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