Abstract Submitted
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Graded-Sequence-of-Approximations: Quantum Mechanical Forces for Molecular Dynamics[1] KEITH RUNGE, Quantum Theory Project, University of Florida, DECARLOS E. TAYLOR, US Army Research Lab, V. V. KARASIEV, S. B. TRICKEY, FRANK E. HARRIS, Quantum Theory Project, University of Florida — The rate-limiting step in the multiscale simulation of materials, biomolecular, and other complex systems is quite generally the generation of the quantum mechanical (QM) forces in the chemically active region. A sequence of approximations involving both QM and classical approximations is used to reduce the computational intensity of the problem. More computationally intensive approximations of greater accuracy, are used at infrequent simulation steps to recalibrate forces from the less intensive calculations, which have lesser accuracy. The graded-sequence-of-approximations technique is illustrated in a particularly demanding case in which we have used a published classical potential for silica with QM forces generated by a quantum chemical technique independently trained to reproduce relevant coupled-cluster forces.

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