Abstract Submitted
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Quantum and Classical Electrostatics Among Atoms[1] T. P. DOERR, O.I. OBOLENSKY, A. Y. OGURTSOV, YI-KUO YU, National Center for Biotechnology Information — Quantum theory has been unquestionably successful at describing physics at the atomic scale. However, it becomes more difficult to apply as the system size grows. On the other hand, classical physics breaks down at sufficiently short length scales but is clearly correct at larger distances. The purpose of methods such as QM/MM is to gain the advantages of both quantum and classical regimes: quantum theory should provide accuracy at the shortest scales, and classical theory, with its somewhat more tractable computational demands, allows results to be computed for systems that would be inaccessible with a purely quantum approach. This strategy will be most effective when one knows with good accuracy the length scale at which quantum calculations are no longer necessary and classical calculations are sufficient. To this end, we have performed both classical and quantum calculations for systems comprising a small number of atoms for which experimental data is also available. The classical calculations are fully exact; the quantum calculations are at the MP4(SDTQ)/aug-cc-pV5Z and CCSD(T)/aug-cc-pV5Z levels. The precision of both sets of calculations along with the existence of experimental results allows us to draw conclusions about the range of utility of the respective calculations.

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