Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Real-space pseudopotential methods for calculating the vibrational Stark tuning rate[1] BENJAMIN GARRETT, JAMES CHELIKOWSKY, University of Texas at Austin — We introduce a real-space method based on pseudopotentials constructed within density functional theory for computing the vibrational Stark effect. With wave functions defined in real space and cluster boundary conditions, convergence is controlled solely by the grid spacing. Moreover, charged systems can be incorporated without a compensating background charge. Real space methods also have the advantage that neither polarization functions nor supercells are required to simulate external electric fields. We illustrate this method by calculating the Stark tuning rates of small carbonyls and nitriles. The use of high-order integration techniques allow for a coarser (less expensive) grid spacing. Perturbative methods for determining the tuning rate will also be discussed.

[1]We acknowledge support from the U.S. Department of Energy from grant DE-FG02-06ER46286.

James Chelikowsky
University of Texas at Austin

Date submitted: 05 Nov 2015 Electronic form version 1.4