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Application of Gaussian Approximation Potentials to Barium Titanate JASON VIELMA, GUENTER SCHNEIDER, Oregon State University — The computational study of complex phenomena over long time and distance scales not accessible to first principles calculations requires empirical potentials usually derived by integrating out the electronic degree of freedoms. Recently, a parameter free approach called Gaussian Approximation Potentials (GAP) has been shown that it can duplicate first principles density functional theory (DFT) total energies and atomic forces accurately [1]. In a GAP the atomic neighborhood of an atom is projected onto the angular momentum channels of Wigner-D functions, yielding a bispectrum of the expansion coefficients of the atomic density. A non-parametric Gaussian Process regression is used to fit a database of total energies and forces to the combination of angular momentum channels constituting the bispectrum. We report initial results of using a GAP to describe the ferroelectric perovskite Barium Titanate ($BaTiO_3$).

[1] A. P. Bartok, M. C. Payne, R. Kondor, and G. Csanyi, Phys. Rev. Lett. **104** 136403 (2010).

Guenter Schneider
Oregon State University

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