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# MINFF: A new atomistic forcefield for molecular simulations of minerals

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Classical and mechanistic molecular simulations such as Monte-Carlo and Molecular dynamics simulations have become a regularly used technique to obtain detailed insights into the structure, dynamics and thermodynamics of a variety of geochemical systems. The predictive power of such simulations relies however on the accuracy of pre-defined and generalized mechanistic forcefields.

This research presents a family of entirely new general and tailor-made forcefields parameters called MINFF[1], which incorporates (covalent) angle constraints to maintain accurate bonding distances, angles and overall unit cell metrics. The development of this new forcefield was motivated by the need to improve structural and vibrational data between experiments and simulations using existing forcefields such as CLAYFF and the INTERFACE FF[2,3], as revealed from the analysis of vibrational properties, Bond Valence Sum (BVS) data and comparison of experimental/theoretical XRD diffractograms. New atomtypes also enable the simulation of a wider range of minerals than currently possible with existing forcefields.

The forcefield optimization was performed via iterative MD simulations in Gromacs, using a Levenberg–Marquardt routine and the atom toolbox in MATLAB[4]. All simulations used a single type of angular constraint (0, 250, 500, 1500 $kJ{\cdot}mol^{-1}{\cdot}rad^{-2}$) for all M-O sites (M being Al, Mg, Si, Fe, Ca), but fixed DDEC6 partial charges. Optimization was made both synchronously for over 30 hydroxide/oxide and clay minerals (general MINFF) as well as independently (tailor-made MINFF), and targeted the Lennard-Jones parameters by minimizing the weighted residuals from differences in bonds, angles and unit cell metrics. Although the results from this study applying new angle constraints to both CLAYFF and MINFF forcefields, show significant improvement in the unit cell metrics and atomic positions of many types of common layered and non-layered (hydr)oxides minerals, it also questions the actual benefit of using generalized forcefields versus mineral specific and tailor-made forcefields.

[1] Holmboe, M., MINFF repository., Web:github.com/mholmboe/minff

[2] Cygan, R.T., Liang, J.J., & Kalinichev, A.G., Journal of Physical Chemistry B., 108(4), 1255–1266, (2004).

[3] Heinz, H., Koerner, H., Anderson, K.L., Vaia, R.A., & Farmer, B.L., Chemistry of Materials., 17(23), 2005,

[4] Holmboe, M., Clays and Clay Minerals., 67(5), 419–426, 2019.