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Article

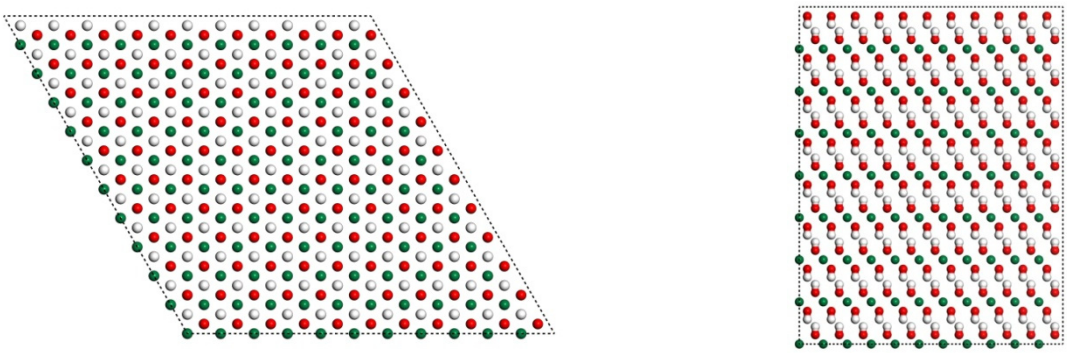
Equation of State, Compressibility, and Vibrational Properties of Brucite over Wide Pressure and Temperature Ranges: Atomistic Computer Simulations with the Modified ClayFF Classical Force Field

Evgeny V. Tararushkin [1], Vasily V. Pisarev [1,2] and Andrey G. Kalinichev [3,*]

[1] International Laboratory for Supercomputer Atomistic Modelling and Multi-Scale Analysis, HSE University, 123458 Moscow, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, 125412 Moscow, Russia
[3] Laboratoire SUBATECH (UMR 6457–IMT Atlantique, Nantes Université, CNRS/IN2P3), 44307 Nantes, France
* Correspondence: kalinich@subatech.in2p3.fr

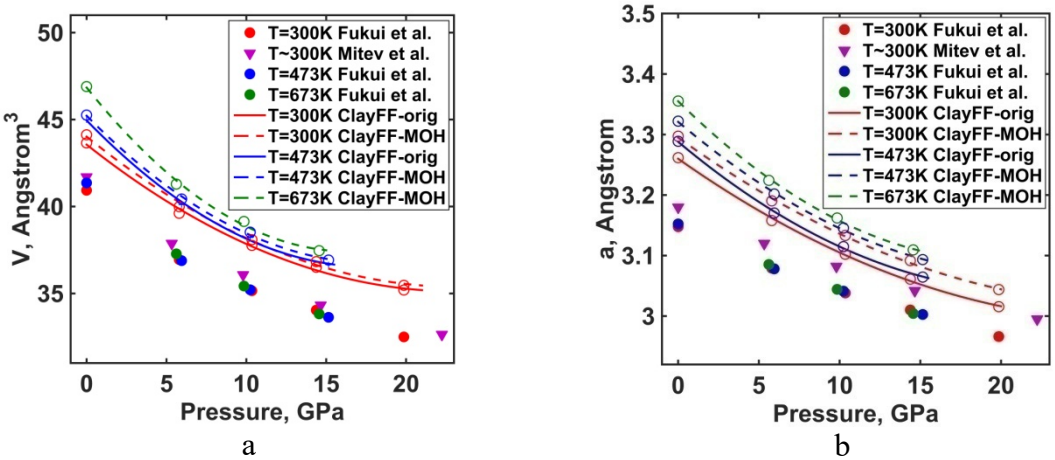
Electronic Supplementary Material

Figures S1–S7



a b

Figure S1. Two projections of the brucite simulation supercell. **a** looking along the *c* axis; **b** looking along the *b* axis. Green atoms–Mg, red atoms–O, white atoms–H.



a b

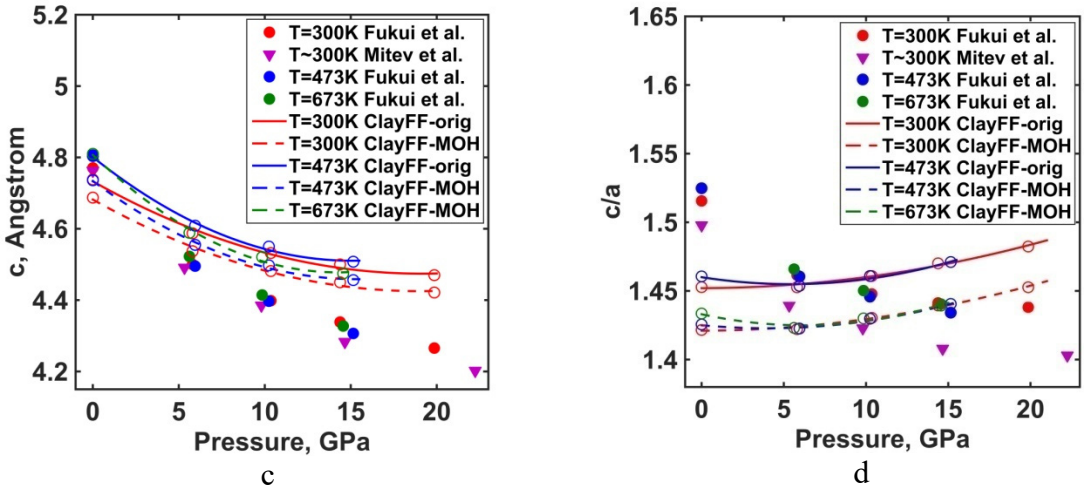


Figure S2. a Volume of the unit cell for brucite as function of pressure; **b** pressure dependence of the parameter *a* of brucite; **c** pressure dependence of the parameter *c* for brucite; **d** ratio of unit cell parameters *c*/*a* for brucite as a function of pressure. Experimental data of Fukui et al. [1], and Mitev et al. [2] are shown as symbols.

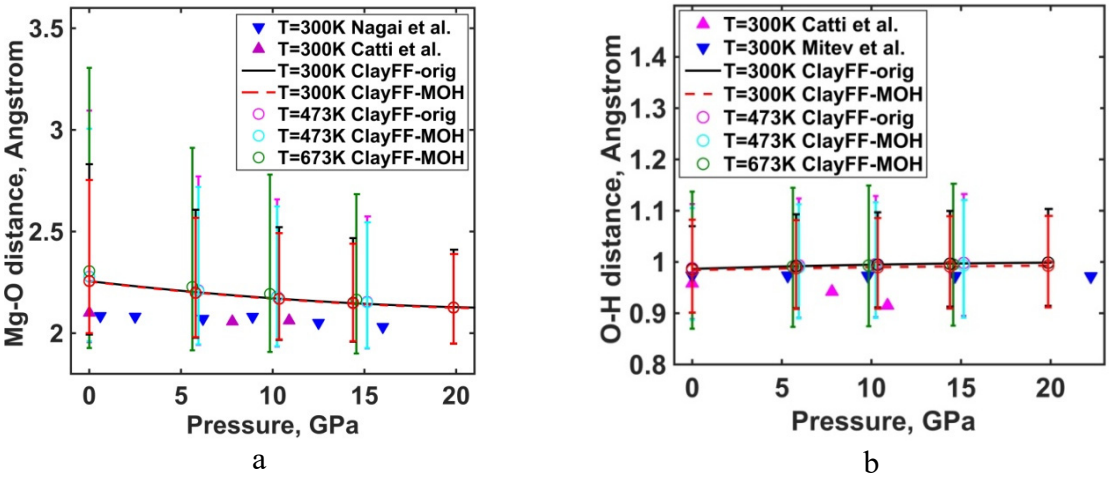


Figure S3. a Pressure dependence of the simulated Mg–O distances in [MgO_6] octahedra; **b** pressure dependence of the simulated O–H distances in structural hydroxyls. Experimental data of Nagai et al. [3], Catti et al. [4], and Mitev et al. [2] are shown as symbols.

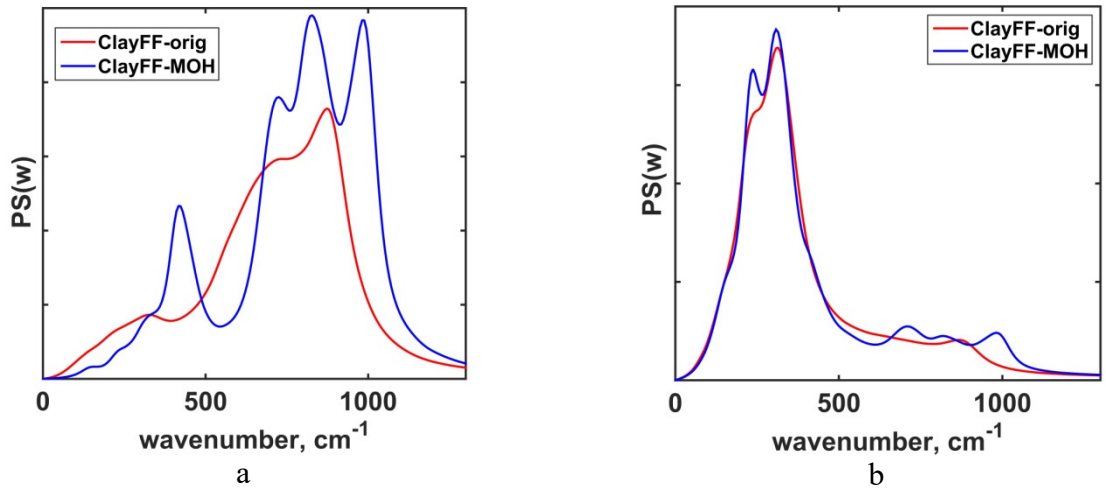


Figure S4. Power spectra for H_{xy} (**a**) and O_{xy} (**b**) for both versions of the ClayFF force field.

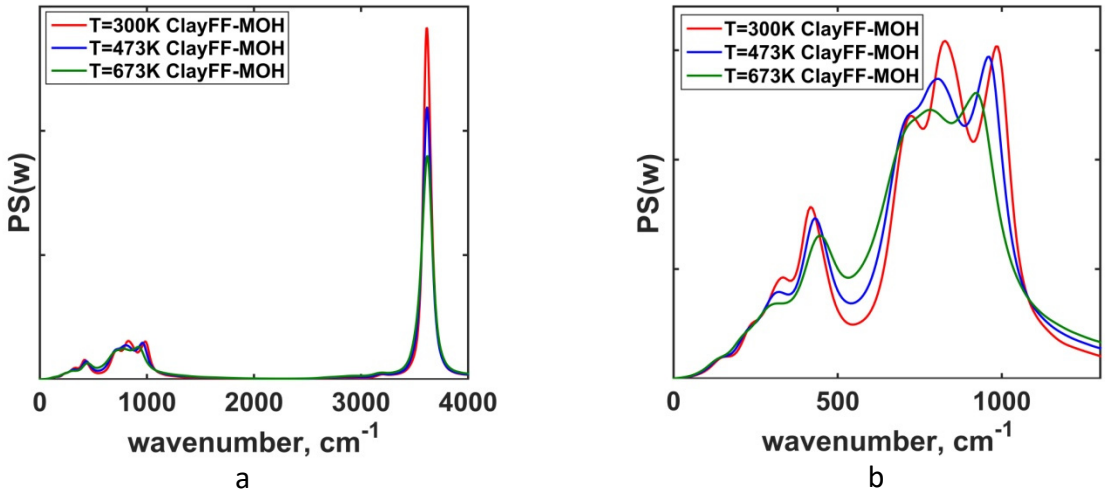


Figure S5. Power spectra of brucite at P=1 bar and high temperatures for the ClayFF-MOH model. **a** entire spectral range of atomic vibrations; **b** librational modes.

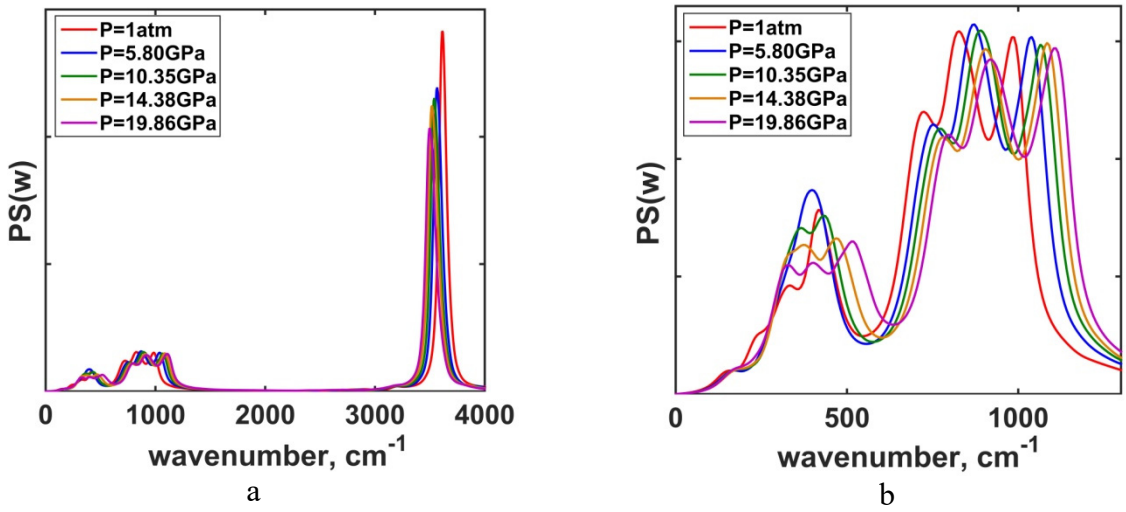


Figure S6. Power spectra of brucite at T=300 K and high pressures for the ClayFF-MOH model. **a** entire spectral range of atomic vibrations; **b** librational modes.

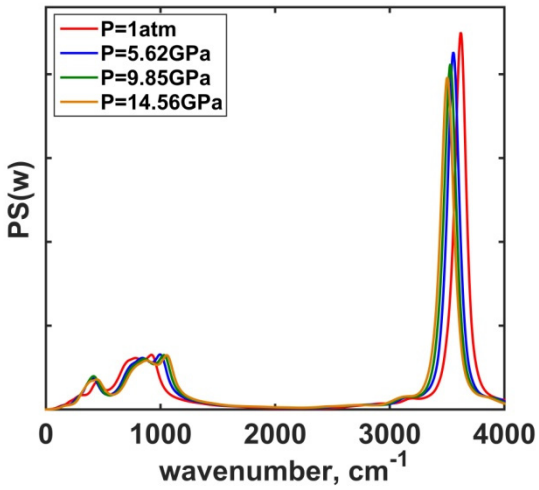


Figure S7. Power spectra of brucite at *T*=673 K and high pressures for the ClayFF-MOH model.

References

1. Fukui, H.; Ohtaka, O.; Suzuki, T.; Funakoshi, K. Thermal expansion of $Mg(OH)_2$ brucite under high pressure and pressure dependence of entropy. *Phys. Chem. Minerals* **2003**, *30*, 511–516. https://doi.org/10.1007/s00269-003-0353-z
2. Mitev, P. D.; Gajewski, G.; Hermansson, K. Anharmonic OH vibrations in brucite: Small pressure-induced redshift in the range 0-22 GPa. *Amer. Mineral.* **2009**, *94*, 1687–1697. https://doi.org/10.2138/am.2009.3188
3. Nagai, T.; Ito, T.; Hattori, T.; Yamanaka, T. Compression mechanism and amorphization of portlandite, $Ca(OH)_2$: Structural refinement under pressure. *Phys. Chem. Minerals* **2000**, *27*, 462–466. https://doi.org/10.2138/am-2000-5-615
4. Catti, M.; Ferraris, G.; Hull, S.; Pavese, A. Static compression and H disorder in brucite, $Mg(OH)_2$, to 11 GPa: a powder neutron diffraction study. *Phys. Chem. Minerals* **1995**, *22*, 200–206. https://doi.org/10.1007/BF00202300