

## Publikationen

(2020): Hartree-Fock simulation of hematite surfaces with a posteriori calculation of correlation energy. Preisträgervortrag zur Verleihung des Georg-Simon-Ohm-Preises der Deutschen Physikalischen Gesellschaft an David Scholz. In: DPG-Frühjahrstagung, Dresden (abgesagt wegen Covid-19, gehalten an THD), Dresden.

(2020): Convergence of surface energy calculations for various methods: (001), (012), (100) hematite and the applicability of the standard approach. In: Journal of Physics: Condensed Matter, vol. 32, no. 18. DOI: 10.1088/1361-648X/ab6f88.

(2019): Convergence of surface energy calculations for various methods: (0 0 1) hematite as benchmark. In: Journal of Physics: Condensed Matter, vol. 31, no. 19. DOI: 10.1088/1361-648X/ab069d.

(2018): Ab initio simulation of structure and surface energy of low-index surfaces of stoichiometric alpha-Fe<sub>2</sub>O<sub>3</sub>. In: Surface Science, vol. 671, no. May, pp. 11-16. DOI: 10.1016/j.susc.2018.01.010.

(2017): Hartree-Fock simulation of the (0 0 0 1) surface of hematite with a posteriori calculation of the correlation energy. In: Computational Materials Science, vol. 137, no. September, pp. 340-345. DOI: 10.1016/j.commatsci.2017.06.011.