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High-Throughput study of chemical substitution in clay minerals PRIYA GOPAL, Central Michigan University, MI, , MARTA GUSMAO, Federal University of Amazonas, Manaus, Brazil, ANDREW SUPKA, Central Michigan University, MI, MARCO FORNARI, Central Michigan University, MI,, MARCO BUONGIORNO NARDELLI, University of North Texas, Denton TX —
High-throughput (HT) DFT computations facilitates the understanding and the design of materials with novel properties. In this work, we use our HT infrastructure, AFLOWπ, to compute the electronic structure and related properties for mineral in the clay family: lizardite ($Mg_3(Si_2O_5)(OH)_4$), talc ($Mg_3(Si_2O_5)_2(OH)_2$), kaolinite($Al_2(Si_2O_5)(OH)_4$) and pyrophyllite ($Al_2(Si_2O_5)_2(OH)_2$). Using these four prototypes, we studied the effect of chemical substitutions in 48 different compositions. We computed the formation energies, optimal lattice parameters, elastic constants and the band structures using ACBN0, a pseudo hybrid Hubbard density functional, all of which is incorporated in the AFLOWπ framework. One main result shows that Ni-substituted lizardite ($Ni_3(Si_2O_5)(OH)_4$) is structurally stable and is a promising candidate in spintronic applications as spin filter.

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