Modelling electron structure of double halide perovskites doped with transition metals

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Conventional DFT calculations of band structures and density of states in highly heterogeneous doped supercells are computationally expensive. This work proposes an evolutionary framework for host–dopant compound design along with recommended parameters for efficient DFT validation. A hybrid parallel genetic algorithm [1] combining an island model for rival generations' creation and slave-master model for highly efficient parallel fitness evaluation was deployed. It implemented machine-learning derived Bartel tolerance factor [2], dopant-host Shannon radii relation and band gap prediction with graph networks [3-4] for fitness calculations. Most prospective candidates of double halide perovskites for doping with transition metals to achieve broadband NIR emission had their band structures and projected density of states evaluated using spin-aware DFT+U [5-7]. Finally, discussion of results and an outline for future work is presented.

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