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Tuning of Metal-Metal Bonding by Counterion Size in Hypothetical AETiO₂ Compounds XIAODONG WEN, ROALD HOFFMANN, Department of Chemistry and Chemical Biology, Cornell University, Ithaca, NY — The structures and electronic properties of a number of real and hypothetical ABX₂ compounds sharing (or evolving from) a single P4/mmm structural type are examined utilizing first principle calculations. These include the known CaCuO₂ and SrFeO₂ phases. A number of variations of this P4/mmm ABX₂ framework, some obvious, some exotic, all with a chemical motivation, were investigated: A=alkali metal, alkaline earth metal or La, B= Ti, Fe, Cu or Pt, and X=C, O, S, C₂, H₂ or F. Careful attention was given to the d-orbital splitting patterns and magnetic states (ferromagnetic or antiferromagnetic) of these compounds, as well as their stability gauged by phonon dispersions and energetics. The most interesting as yet unmade compounds that emerged was an AETiO₂ (AE = alkaline earth metal, Be, Mg, Ca, Sr and Ba) series, with Ti-Ti bonding, part σ , part π , tuned by the AE²⁺ cation size. The Ti-Ti bonding in 3D AETiO₂ structures has a unique electronic feature of 1D metal chain. These AETiO₂ (M=Ca, Sr and Ba) structures are calculated to be thermodynamically and dynamically stable. Experimentally, the high temperature method fails so far. Perhaps a low temperature method offer a better pathway to synthesize the AETiO₂ (M=Ca, Sr and Ba) structures.

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