Abstract Submitted
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Inspecting ∼700 A_2BX_4 compounds for energy applications: sorting their ∼40 crystal structures by diagramatic orbital radii maps without energy minimization[1] XIUWEN ZHANG, ALEX ZUNGER, National Renewable Energy Laboratory, Golden, CO 80401 — The A_2BX_4 family of compounds covers ∼44 different crystal structure types and manifest a wide range of physical properties, including ferromagnetism, ferroelectricity, transparent conductivity, as well as superconductivity. We describe here a diagrammatic separation of the different crystal structures of ∼688 A_2BX_4 compounds by plotting a $R_A = R_s(A) + R_p(A)$ *vs* $R_B = R_s(B) + R_p(B)$ map, where R_s and R_p are the s and p "orbital radii" of the neutral, free atoms, previously determined from first-principles pseudopotential theory. We find a 98% successful separation of 688 A_2BX_4 compounds into 44 structure types. Applying this approach to separate Normal from Inverse spinel structures, we find a 96% successful separation for 230 spinels known. These success rate using first-principles orbital radii uniformly exceed the success rates using classic radii (e.g Shannon's crystal radii; Pauling's covalent radii) or Pettifor's numbers. Once the separation maps was constructed, the crystal structure of a new chemical compound can be predicted by placing its R_A and R_B values in the map.

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