Inspecting \( \sim 700 \) \( \text{A}_2\text{BX}_4 \) compounds for energy applications: sorting their \( \sim 40 \) crystal structures by diagramatic orbital radii maps without energy minimization\(^1\) XIUWEN ZHANG, ALEX ZUNGER, National Renewable Energy Laboratory, Golden, CO 80401 — The \( \text{A}_2\text{BX}_4 \) family of compounds covers \( \sim 44 \) 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 \( \sim 688 \) \( \text{A}_2\text{BX}_4 \) 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 \( 688 \) \( \text{A}_2\text{BX}_4 \) 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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