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Electronic structure and bonding in fluorapatites crystals:
 $A_{10}(\text{PO}_4)_6\text{F}_2$ ($A=\text{Ba, Ca, Pb}$ and Sr)¹ CLAUDIA LOYOLA, Universidad Andres Bello, EDUARDO MENENDEZ-PROUPIN, Universidad de Chile, KRISHNA RAJAN, Iowa State University — In this work we report a computational study of electronic properties of fluorapatites ($A_{10}(\text{PO}_4)_6\text{F}_2$ with $A=\text{Ba, Ca, Pb}$ and Sr) using ab initio calculation. We employed Density Functional Theory using a Plane Wave basis set and pseudopotentials to obtain the band structure, total and partial density of states, electronic charge density and electron localization function. We obtain that Ba-, Ca- and Sr-fluorapatite have a wide band gap in the range of ~ 5.4 eV, while the Pb-fluorapatites have a band gap of ~ 3.8 eV and different band structure compared with the rest of fluorapatites. The electron charge density and the electron localization function reveal covalent character of the bond between the oxygen and phosphorus in the tetrahedral substructure for all fluorapatites. We analyze the results and possible causes behind the differences in the electronic structure of these fluorapatites.

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Joaquin Peralta
Universidad Andres Bello

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