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Energy Band Gap Behavior as a Function of Optical Electronegativity for Semiconducting and Insulating Binary Oxides[1] KRISTEN DAGENAIS, University of Maryland, Baltimore County, MATTHEW CHAMBERLIN, COSTEL CONSTANTIN, James Madison University — A relationship between energy band gap and electronegativity has long been understood to exist. However, defining the relationship between the two for binary oxide systems has proven difficult. Many scientists tried to model the band gap as a function of Pauling electronegativity values, but we show that by using a new concept called "optical electronegativity" one can obtain much better predictions regarding band gaps of new oxide. Interestingly we found that the behavior of oxides varies across depending on the chemical group the cation is from. With that knowledge, we developed two equations to describe the alkali earth metal and poor metal oxide. By using our models, we are able to predict the band gap of radium oxide at 5.36 eV. Due to the contributions of 'd' and 'f' orbitals we could not model lanthanide rare earth and transition metal oxides but rather we found that band gaps for both lay beween 3.56 - 5.72 eV, and 1.82 – 3.82 eV, respectively.

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