Invited Speaker

THE CHEMICAL BOND OVERLAP PLASMON AS A TOOL FOR QUANTIFYING COVALENCY IN OPTICAL SOLID STATE MATERIALS

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Correlations between the characteristics of the chemical bond and the properties of matter have long been the subject of intense investigation. In an attempt to get deeper insights on covalency in the special case of lanthanide compounds, we have introduced the concepts of chemical bond overlap polarizability (OP) and ionic specific valence (ISV) [1]. Several consequences of these concepts have been then explored and tested in different systems from diatomic to complex molecules and solids. Among these consequences are the definition of a quantitative covalent fraction scale and a description of ligand field effects in terms of a contact potential that may be treated non phenomenologically when the charge factors, appearing in the Simple Overlap Model, are identified with the ligating atoms ionic specific valences [1,2]. The OP and ISV concepts have also been explored in a more general context. Relevant questions can be raised on possible relationships between macroscopic properties of materials and these concepts. Thus, for example, a good correlation has been found between the non-linear index of refraction (n_2) and the OP [3]. A proposal in which the overlap region is regarded as a localized plasmon-like charge distribution - the chemical bond overlap plasmon (CBOP) - characterized by the OP, has raised the question on the possibility of absorption and inelastic scattering of radiation, above the first ionization threshold, by the overlap region [4]. Predicted CBOP oscillator strengths, scattering and electron energy loss cross sections for solid alkali-halides and aluminum oxides are considerably high and could be measured experimentally. These spectroscopic quantities depend on the OP and ISV, and are suggested as a useful tool for quantifying covalency in optical materials.

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