Computer modeling of the crystallographic structure and defects formation in the Li2WO4, La2(WO4)3 and LiLa(WO4)2

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In the last decade, the alkali rare earth double tungstates ALn(WO4)2 (A=Li, Na, K and Ln = La-Lu) have been intensively investigated concerning their optical properties as laser hosts. Specially, the ones showing tetragonal scheelite-like structure are interesting as solid state laser hosts because of their disordered structure leads to the broadening of the absorption and emission bands. This behavior improves the diode pumping power efficiency in the laser operation as well as the possibility to have a tunable laser system. These materials doped with Nd3+ ions are good candidates for laser hosts in the near-infrared range. In particular, the LiLa(WO4)2 (LLW) compound melt in relatively low temperature and do not show polymorphic transitions upon cooling allowing the growth from the melt. Regarding the low-cost investigation of these materials the computer modeling is a useful technique for determination of the defect properties of materials and the location of dopant ions to optimize the experimental conditions to obtain single crystals for optical applications. Computer modeling methods, based on energy minimization and the Mott-Littleton approach, with interactions represented by interatomic potentials, have been used for determination of the defect properties of materials and the location of dopant ions. Such calculations enable predictions to be made of the sites occupied by dopants, and the form of charge compensation adopted, if needed. The formation energies and solution energies were then calculated for the extrinsic defects (Ln3+ doping), via solid state reactions just for the LLW matrix. The formation energies are also used in a set of equations that can predict the effect of solubility and concentration of dopants in this matrix. These theoretical results are being compared with experimental data for validating this investigation. This work is partially supported by FAPESP, CNPq and CAPES.