
Tellurium oxide based glasses: establishing of nonlinear optical properties from *ab initio* calculations

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Abstract

During the last decades, nonlinear optical materials with high third-order nonlinear optical susceptibility, like tellurium oxide based glasses, have received much attention because they have new photonic device possibilities for applications in optical memory storage, logic and switching.

Since the beginning of this century, a substantial amount of researches was devoted to nonlinear optical properties of various tellurium oxide based glasses of various compositions. In a first step, our aim was to reproduce the experimental data by mean of *ab initio* calculations and to gain a better insight into the origin of the remarkable nonlinear optical properties of those materials. For achieving these purposes, we applied a comprehensive *ab initio* calculation program based on several computational methods and selected the most efficient ones on.

Our concern is now to develop a tool able to establish the nonlinear optical properties of unstudied systems in order to select the most promising ones in preparation for applications. Among the different potential *ab initio* calculation methods we decided to start with molecular calculations on clusters containing terminal hydrogen atoms (TenOmHp). The addition of another metal (like Ti, Zn, Mg...) was planned as a second step once consistent results are observed for the TenOmHp clusters. Several functional and basis sets were tested and the first results are presented on this poster.

Keywords: tellurium oxide, nonlinear optical properties, computer simulations

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