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Nonlinear Optical Properties of TeO_2 Crystals from First Principles

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Since the discovery of their exceptional nonlinear optical coefficients, tellurium-based glasses arouse a very great interest. Their 3rd order non linear susceptibilities are indeed among the highest values observed for glass oxides (20 to 50 times greater than silica) and they thus are potential candidates in the field of long distances transmissions (particularly in the case of immersed systems). **[1]**

The origin of the high values of the non linear indices is classically attributed to the hyperpolarizability of the electronic lone pair present on the tellurium (IV) atom **[2].** However the influence of the structure, in particular at short and medium range is not yet fully understood. For clarifying this point, we wish to study theoretically the effect of an electric field on those compounds.

As the structure of tellurium-based glasses is not easy to determine because of the very singular crystal chemistry of tellurium that frequently adopts TeO_3, TeO_4 or TeO_5 configurations, the only theoretical studies published up to now are focussing on the microscopic nonlinear indices of tellurium oxide molecules of various sizes and geometries.**[3]** Those studies carried on in the framework of the density functional theory (DFT) led to interesting conclusions about the role of the Te-O-Te bridges and their symmetry on the hypersusceptibilities.

Very recently, finite electric field approaches**[4]** have been implemented in DFT programs, allowing to apply an electric field on a crystal unit cell without loosing the periodicity of the calculation. As an alternative to the study of the tellurium oxide molecules, we plan now on studying the TeO_2 polymorphs from the point of view of the macroscopic nonlinear indices.

For this purpose, we use the quantum mechanical code SIESTA 2.0 **[5]** in which we have implemented the finite field scheme. Once established, the reliability of the method, the results on the three TeO_2 polymorphs (α , β and γ) will be exposed. As the tellurium is in different oxygen environment in the three phases, we should be able to shed light on the importance of the structure on the hypersusceptibilities.

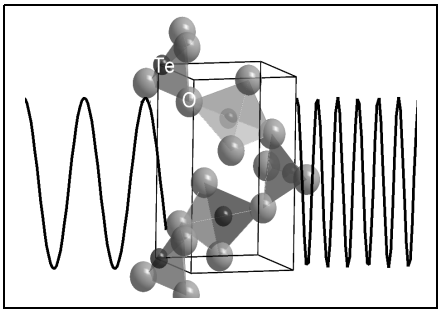

Figure 1: Illustration of nonlinear optics.

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