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Correlations between structural and optical properties of peroxy bridges from first principles

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Interest for oxide glasses has been renewed mainly by increased needs for improved sensors and oxide based resistive random access memories – OxRRAM. In both applications, oxygen and diffusing species or oxygen related defects are expected to play a key role. This work aims at addressing the issue of the optical signature of peroxy bridges by using first-principles methods that combine Density Functional Theory (DFT), GW and the solution of a Bethe-Salpeter Equation (BSE) on a bulk amorphous SiO_2 model. Results show that the presence of bridges induces broad and weak absorption bands between 3.2 and 7.5 eV. By analyzing the correlations between Si-O-O-Si dihedral angle distributions and the corresponding electronic structure, we show that weak and broad absorption origin from low overlap between O-2p states and the further spread of the signal caused by dihedral angle site-to-site disorder. Moreover, the energy difference between the two first optical transitions depends linearly on the energy difference between the two first occupied defect-induced electronic states, i.e. depends on the dihedral angle of the bridge. This behavior may form a basis for explanation of the longstanding controversy regarding the optical signature of peroxy bridges in amorphous SiO_2. As the correlation is independent on the specific hosting hard material, the results apply whenever the dihedral angle of the bridge has some degree of freedom.

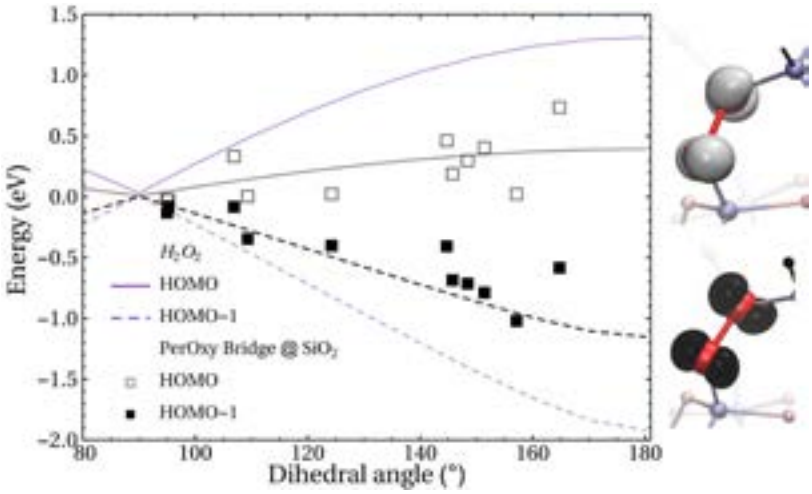

Fig 1: Energy variation of HOMO-1 and HOMO as a function of dihedral angle

Biography

Blaž Winkler is a 3rd year joint PhD student of Physics at University of Nova Gorica, Slovenia, and Optics/Photonics at University Jean Monnet Saint-Etienne, France. His research combines state of the art numerical methods for structural, electronic and optical properties with established experimental procedures to understand the effect of excess oxygen on point defects in amorphous silicon dioxide (silica).

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