

Abstract Submitted  
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**Computational spectroscopy of nanocomposites**<sup>1</sup> MARCO GOVONI, TUAN ANH PHAM, GIULIA GALLI, Department of Chemistry, University of California Davis — Most of the first principles calculations of the opto-electronic properties of nanoparticles appeared in the literature were conducted using structural models of isolated particles. However experiments are carried out on nanocomposites, e.g. nanoparticles in solution or embedded in solid matrices. Recent ab initio studies [1,2] pointed at the importance of taking into account interactions between nanoparticles and the environment surrounding them, in order to provide sensible predictions of their electronic properties, as well as interpretation of experiments. Here we report calculations of the relative position of energy levels of Si nanoparticles embedded in amorphous matrices, as obtained using many body perturbation theory, at the GW level. Our calculations were carried out using a newly developed method to obtain quasi particle energies, based on the spectral decomposition of the dielectric matrix [3].

[1] T.S.Li, F.Gygi and G.Galli *Phys. Rev. Lett.* 107, 206805 (2011)

[2] M.Govoni, I.Marri and S.Ossicini *Nature Photonics* 6, 672 (2012)

[3] H-V.Nguyen, T.A.Pham, D.Rocca and G.Galli *Phys. Rev. B* 85, 081101(R) (2012)

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