
SCIENCE COLLEGE SEMINAR SEMINAR DES COMPUTATIONAL MATERIAL SCIENCE

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Optical properties of nanostructures from empirical pseudopotentials and configuration interaction

In this presentation, I will outline the framework of the empirical pseudo potentials and the configuration interaction methods [1] we use to obtain quantitative predictions of the excited state properties of semiconductor nanostructures. The methodology can be used to describe colloidal nanostructure of few hundred atoms all the way to epitaxial structures requiring millions of atoms. We will illustrate the capability of the method by recent applications [2].

[1] G. Bester, J. Phys.: Condens. Matter. 21, 023202 (2009).

[2] R. Singh and G. Bester. Phys. Rev. Lett 104 196803 (2010); Phys. Rev. Lett 103 063601(2009)

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