## O.25 Automating ΔSCF computations of point defects using AbiPy workflows

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Simulating luminescent properties of points defects requires to build large supercells to reduce spurious interaction between periodically repeated images. This hinders the use of Bethe-Salpeter equation to characterize the excited state. One can alternatively use the ΔSCF method, whereby the eigenfunction associated to the highest occupied state of the ground state is constrained to be unoccupied while the next energy state is constrained to be occupied. Transition energies are then computed as difference of two total energies. Although not formally exact, this method yield reasonable agreement with experiment [1]. One can also predict the shape of the emission/absorption spectrum by analysing the atomic displacements induced by the electronic transition [2].

In this talk, I will first describe how the ΔSCF method can be used with ABINIT by taking the example of substitutional defect in Europium-doped luminescent materials. I will then present 'LumiWork', an ongoing project aiming at using AbiPy workflows to automate most of the error-prone steps of the methodology. The goal is to provide a general framework allowing the computation of luminescent properties of point defects. Before considering large-scale computations of such properties for varieties of materials, serious challenges must be addressed: How to deal with capricious SCF cycles convergence in the excited state, how to choose the supercell size, how to deal with multiple substitutional sites,... These points will be briefly discussed. Finally, AbiPy post-processing tool allowing to analyze the data produced by a 'LumiWork' will be presented.

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[1] Yongchao Jia et al., First-principles study of the luminescence of $Eu^{2+}$ -doped phosphors, Physical Review B **96**, 125132 (2017).

[2] Julien Bouquiaux et al. Importance of long-range channel Sr displacements for the narrow emission in $Sr[Li_2Al_2O_2N_2]$: $Eu^{2+}$ phosphor. ArXiv preprint arXiv:2010.00423 (2020).