Projecte per beques d'estiu 2017

Dades del projecte:

Títol:	Design of optimal tuned hybrid functionals for the evaluation of nonlinear optical properties: Atomic and diatomic decomposition of nonlinear optical properties.
Supervisor:	Dr. Pedro Salvador i Dr. Josep Maria Luis
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Grup de recerca:	QTMEM
Destinat a estudiants:	4t any
Lloc de treball:	Fac. Ciències
Places ofertes:	1 (4t any)
Data d'inici:	a concretar amb l'estudiant
Data d'acabament:	a concretar amb l'estudiant
Seguiment:	Diària

Coneixements específics que ha de tenir l'estudiant: Coneixements de Química Teòrica i Computacional adquirits durant els cursos de segon, tercer i quart de grau.

Estudis en curs requerits: Química

Formació que adquirirà l'estudiant en realitzar aquesta activitat: Aprenentatge i formació en les tècniques computacionals utilitzades per la determinació de les propietats òptiques no lineals i per la descomposició de l'energia i propietats moleculars fent servir cel·les de Voronoi topològiques difuses (TFVC) utilitzant el programa (QTAIM). El candidat treballarà en un equip format per diversos estudiants, per la qual cosa l'aprenentatge serà cooperatiu i també es formarà al candidat en les competències del treball cooperatiu.

Descripció de l'activitat que ha de fer l'estudiant: Great attention has been paid to the materials characterized by a large nonlinear optical (NLO) response, as they are commonly used in optical communication technology. In the particular case of the evaluation of NLO properties (NLOP) of oligomers and molecular chains, the DFT methods overestimate by several order of magnitude the exact values. The main reason behind DFT failure in the calculation of the NLOP is the "short-sightedness" of the exchange-correlation potentials. The tuned hybrid functionals can remedy this situation by including the optimal percentage of exact exchange. The first goal of the present project focuses on designing new tuned hybrid functional that provide a correct description of NLOP. Overcoming one of the most important DFT pitfalls, promises to furnish new DFT functionals with the flexibility to accurately describe a wider range of properties, paving the way towards the development of all-purpose functionals. The NLOP will be computed for $(H_2)_n$ and polyacetylene chains for different percentages of the exact exchange. First, the functionals will be calibrated using benchmark NLOP results obtained with post-HF methods. It will be studied the dependence of the optimal tuning factor with the chain size and with the chemical system. Furthermore, it will be analyzed the NLOP obtained with several attenuating parameters decomposing the properties in atomic and diatomic contributions. We will also compare the decompositions obtained using the topological fuzzy Voronoi cells (TFVC) atomic partition scheme as implemented in APOST-3D program, and Quantum Theory of Atoms in Molecules (QTAIM) domains obtained using AIMall. This analysis will deepen and facilitate the understanding of the improvement in performance of NLOP calculations by the optimal tuned hybrid functionals.