

VISTA Seminar

Seminar 33

March 16, 2021

**10:00 am – 11:30 am EST / 3:00 – 4:30 pm GMT / 4:00 pm – 5:30 pm
Paris**

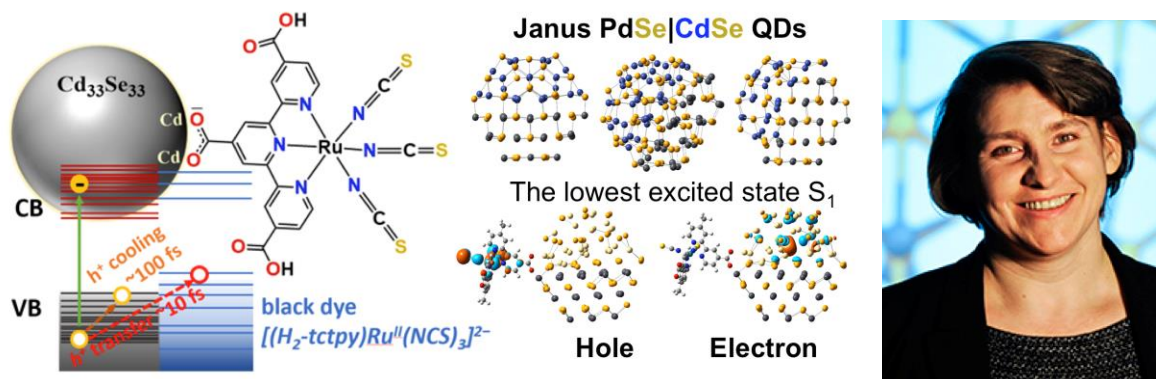
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Modeling Charge Transfer in Quantum Dot/Dye Nanocomposites

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Recent focus on assemblies of the quantum dots (QDs) functionalized by various organic and metal-organic dyes is dictated by their promise to serve as a key element for both solar-to-electrical and solar-to-chemical energy conversion processes. In both types of applications, conditions and mechanisms of the charge transfer from the photoexcited QD to the dye or backward play a crucial role in the device performance. Applying non-adiabatic molecular dynamics (NAMD) and the Fewest Switching Surface Hopping (FSSH) methods, we have revealed ultrafast hole transfer (~ 10 fs) from the CdSe QD to the Ru(II) black dye, following by a slow component (~ 100 fs) associated with the redistribution of population throughout QD states in the energy range of the initial excitation. As such, our calculations prove the realization of the ultrafast interfacial hole transfer from the photoexcited CdSe QD to the dye, which is rationalized by strong non-adiabatic couplings between the QD surface states and the high frequency vibrations of the isocyanide ligands of the black dye. We also have studied the effect of the complex heterostructures of Janus QDs, where a half of the QD is made from CdSe and another half is from PbSe forming an interface along a specific crystalline direction, which permits more control over the charge transfer processes and the overall efficiency of the energy conversion. We have found that the Pb-enriched (111) crystalline direction of the interface provides a charge-transfer character of lower energy transitions, with an electron more localized on the PbSe surface, while the hole is delocalized over the black dye. Overall, our calculations provide atomistic insights into the surface chemistry of QD-dye composites, which knowledge is needed for controlling charge transfer by means of the QD interface and QD-molecule engineering.

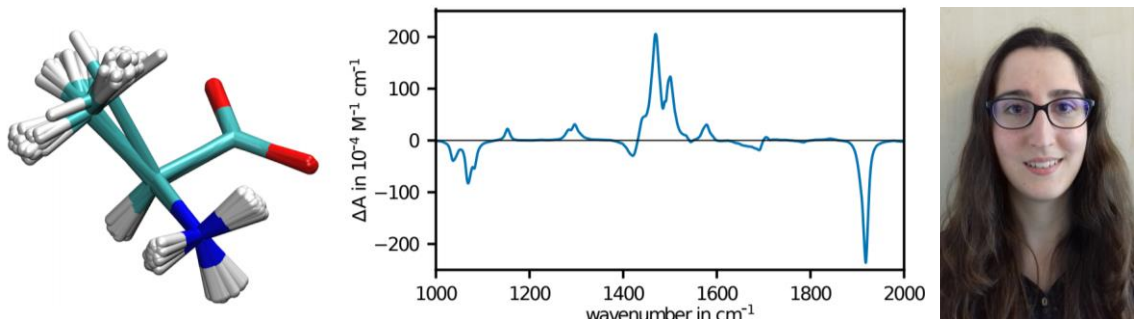
Determination of Vibrational Circular Dichroism spectra of flexible molecules through a classical dynamic approach using polarisable force fields

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Vibrational circular dichroism (VCD) is the weak difference in absorption for chiral molecules between right- and left- polarized light in the infrared range. It has promising applications in pharmacology owing to its ability to determine absolute configurations of chiral molecules. The shape of VCD spectra is highly sensitive to minor changes in conformation and molecular interactions, which makes it a sensitive probe of conformational isomerism and solvation. [1, 2]

As an alternative to methods based on explicit descriptions of electronic structure [3, 4, 5] and to circumvent their limited sampling capabilities in time and space, we have attempted to simulate the VCD spectrum directly from the molecular dynamics (MD) trajectories employing a polarisable force field, extending earlier efforts dedicated to the IR spectrum [6]. In this presentation, we describe our implementation of VCD spectroscopy using the AMOEBA polarisable force field [7] in the Tinker software package [8] and our first applications to solvated amino acids, emphasizing the roles of temperature and the environment on the VCD spectrum. Finally, electric and magnetic dipole moments and vibrational spectra will be evaluated by comparison with first-principles simulations.

References :

- [1] Christian Merten, Robert McDonald, and Yunjie Xu. *Inorganic chemistry*, 53(6):3177–3182, 2014.
- [2] Katia Le Barbu-Debus, Jessica Bowles, Sascha Jähnigen, Carine Clavaguéra, Florent Calvo, Rodolphe Vuilleumier, and Anne Zehnacker. *Physical Chemistry Chemical Physics*, 22(45):26047–26068, 2020.
- [3] Ariel Pérez-Mellor and Anne Zehnacker. *Chirality*, 29(2):89–96, 2017.
- [4] Sascha Jähnigen, Arne Scherrer, Rodolphe Vuilleumier, and Daniel Sebastiani. *Angewandte Chemie International Edition*, 57(40):13344–13348, 2018.
- [5] Katia Le Barbu-Debus, Arne Scherrer, Aude Bouchet, Daniel Sebastiani, Rodolphe Vuilleumier, and Anne Zehnacker. *Physical Chemistry Chemical Physics*, 20(21):14635–14646, 2018.
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- [7] Jay W Ponder, Chuanjie Wu, Pengyu Ren, Vijay S Pande, John D Chodera, Michael J Schnieders, Imran Haque, David L Mobley, Daniel S Lambrecht, Robert A DiStasio Jr, et al. *The journal of physical chemistry B*, 114(8):2549–2564, 2010.
- [8] J. W. Ponder. *TINKER - Software Tools for Molecular Design (version 8)*. <http://dasher.wustl.edu/tinker> (accessed May 26th, 2021).

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Alexey Akimov is inviting you to a scheduled Zoom meeting.

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