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Impact of the steric hindrance of thiol ligands on the optical properties of 2D CdSe semi-conductors

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Semi-conducting nanoplatelets (NPIs) are known as a new category of 2D nanomaterials with promising optical properties. However, recent reports have shown that the thickness breathing modes of CdSe NPIs could be probed by low-frequency Raman scattering. Notably, the effect of an additional mass of organic ligands bounded to the free surface of NPIs has displayed strong deviations of the measured Raman frequencies compared to the expected values. [1] Other studies have pointed out that the nano-mechanical properties of CdSe NPIs could be dependent of the nature of the ligands. By increasing the molecular chain of alkylthiols ligands, great modifications in the vibration frequencies and on the curvature are visible involving a great discrepancy between the mass-load model and the experimental datas. [2]

However, this model does not take into account the structural modification of the ligands. Here we propose to compare the NPIs properties after exchanging the native carboxylates by thiol ligands with similar molecular weight but various conformations. Indeed, the impressive changes observed in TEM and Raman spectroscopy let us think that the steric hindrance of ligands anchored on the surface has a huge influence on both morphology and optical properties of the NPIs. By comparing 1-Octanethiol (OT) and 2-Ethylhexanethiol (EHT), it is clear that the shift-up of the vibration frequency (figure 1c) and the complete unfolding of the platelet are due to the branching position and length on the backbone of the molecule. (Figure1c). All those different effects have to be disentangle in order to improve the consistence of the mass-load model.

[1] A. Girard, L. Saviot, S. Pedetti, M.D. Tessier, J. Margueritat, H. Gehan, B. Mahler, B. Dubertret, A. Mermet, The mass load effect on the resonant acoustic frequencies of colloidal semiconductor nanoplatelets, *Nanoscale* (2016), 8, 13251-13256.

[2] Q. Martinet, J. Baronnier, A. Girard, T. Albaret, L. Saviot, A. Mermet, B. abecassis, J. Margueritat, B. Mahler, Ligand-dependent nano-mechanical properties of CdSe nanoplatelets : calibrating nanobalances for ligand affinity monitoring, *Nanoscale* (2021), 13, 8639-8647.

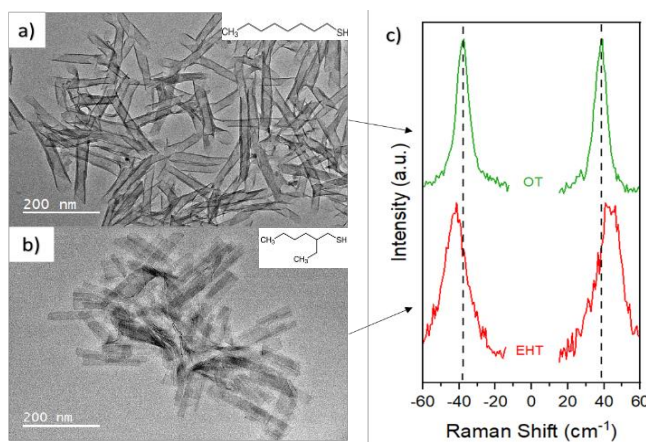


Figure 1: TEM images of 3MLs CdSe Nanoplatelets after typical ligand exchange with: a) 1-Octanethiol, b) 2-Ethylhexanethiol. c) Corresponding low-frequency Raman spectra.