A Universal Database of Surface Ligands in Colloidal Semiconductor Nanocrystals

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Colloidal semiconductor nanocrystals (NCs) combine inorganic materials scaffolds with surface organic ligands. A key role played by the ligands in all these systems is the stabilization of the inorganic region in organic solvents to prevent its dissolution. The suitability of a certain ligand depends on several factors such as magnitude of the NC/ligand binding strength, inter-ligand packing, and ligand/solvent interactions. (1) In practice, each NC type has its best ligand, however finding such ligand is a tedious work, if one considers the labor and material costs involved in the experiments. In this context, computational screening provides an attractive alternative to browse the largely unexplored space of potentially interesting ligands. In this presentation, we introduce a public database of organic molecules, derived by an advanced filtering of the PUBCHEM database, (2) with the aim of building a subset of surface ligands candidates that are potentially suitable to passivate the surface of any inorganic material substrate. For each ligand in the database, we additionally provide relevant chemical and physical properties, from the boiling and melting points to more specific properties that account for the interactions with the solvent. These ligand properties are material-independent and can therefore be used as an orientation tool for ligand-capped inorganic materials research in general. We introduce a public database of organic molecules, derived by an advanced filtering of the PUBCHEM database, (2) with the aim of building a subset of surface ligands candidates that are potentially suitable to passivate the surface of any colloidal semiconductor nanocrystal.

Citazioni

(1) Zito, J., & Infante, I. (2021). The future of ligand engineering in colloidal semiconductor nanocrystals. Accounts of Chemical Research, 54(7), 1555-1564.

(2) Kim, S., Chen, J., Cheng, T., Gindulyte, A., He, J., He, S., Li, Q., Shoemaker, B. A., Thiessen, P. A., Yu, B., Zaslavsky, L., Zhang, J., & Bolton, E. E. (2023). PubChem 2023 update. Nucleic Acids Res., 51(D1), D1373–D1380.