Searching for the best molecular semiconductors

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We present several approaches to screen a large database of molecular materials in search for known compounds with selected optimal properties. This lecture will focus on the balance to be sought between high throughput screening of large databases, bottom-up (physics) modelling and top-down data science approach. We first consider optical properties like (i) finding novel singlet fission materials [1] and (ii) finding novel materials for temperature activated delayed fluorescence. We then consider the even more challenging problem of computing the charge mobility [2] and screening thousands of materials with approximated methods [3]. Finally, we provide examples of using Machine Learning for the discovery of new organic photovoltaic materials, highlighting the opportunities but also the challenging relation with traditional physical sciences [5].

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