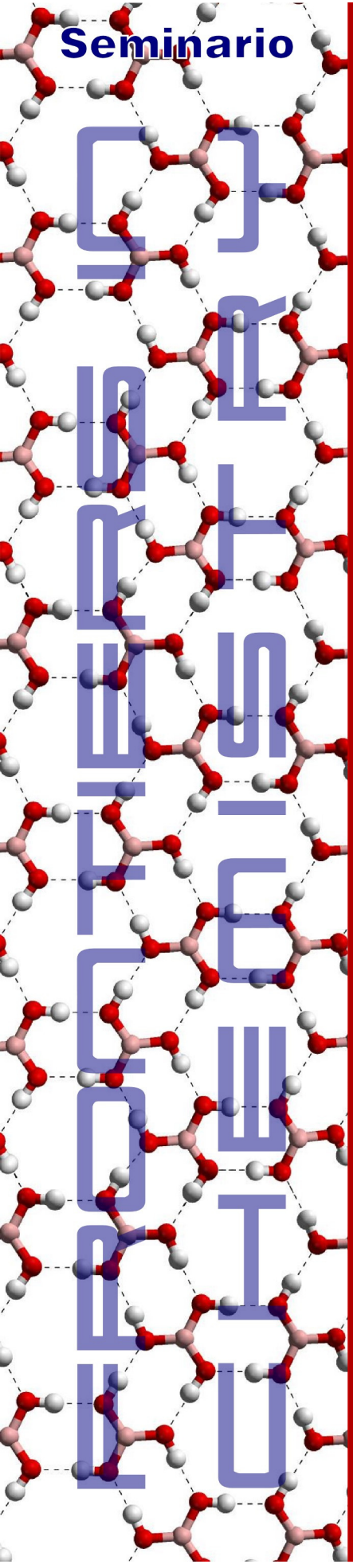

Università degli Studi di Padova
Dipartimento di Scienze Chimiche

Ciclo di Seminari 'Frontiers in Chemistry'

Prof. Alessandro Troisi

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Organic materials for electronics: design by model reduction

Martedì 25 Giugno 2019, ore 14.00
Aula I, Dipartimento di Scienze Chimiche,
Via Marzolo 1 - Padova

The principles of how charge is transported in organic materials (molecular, polymeric) will be reviewed. We then present a common strategy to design new materials for electronics based on the construction of reduced (predictive) models from (detailed) atomistic one. We will argue that, somewhat counterintuitively, our models are more predictive if they contain less details. The topics considered in this lecture include (i) the definition of a map of all organic semiconductors for charge transport; (ii) the desirable properties of electron acceptors in organic solar cells; (iii) derivation of possible design rules for semiconducting polymers; (iv) uses and limitations of machine learning approaches for the same problems; (v) discovery of singlet fission materials via brute force.

La presenza della S. V. sarà molto gradita.

Prof. Michele Maggini
Direttore del Dipartimento di Scienze Chimiche

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