Namur Institute of Structured Matter

UNIVERSITÉ DE NAMUR

Seminar

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« Embedded many-body perturbation theory for the electronic properties of organic systems »

When and where:

Tuesday March 23rd 2021 at 12:50
Online
Teams link: NISM Team, "Séminaires" channel.

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« Embedded many-body perturbation theory for the electronic properties of organic systems »

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Many-body perturbation theories, such as the GW and Bethe-Salpeter formalisms, have become a tool of choice in solid-state physics for studying the optoelectronic properties of crystals. Difficulties arise when attempting to explore with such techniques extended disordered systems: periodic boundary conditions cannot be used while the importance of long-range electrostatic and dielectric effects preclude the quantum chemistry approach of considering isolated molecules in the gas phase. We will present recent developments along the line of embedded, or QM/MM, formalisms allowing to perform accurate many-body calculations for the optoelectronic properties of organic systems immersed in complex electrostatic and dielectric environments. Applications to the study of the elusive doping mechanisms in organic semiconductors and to organic photovoltaics will be presented.