CFEL SCIENCE

SEMINAR

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CFEL-bldg. 99, seminar room III

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Modeling transport in nanostructured materials

Charge transport processes in ‘everyday’ materials rely on a wealth of fundamental physical processes and external influence factors. In large-scale applications such as non-volatile high-density memories, reprogrammable logic devices or illumination panels with organic light emitting diodes the interplay between intrinsic and extrinsic mechanisms may be entwined in a complex manner. Various length and time scales may be involved, rendering a thorough theoretical description cumbersome. Nano-sized systems, in contrast, are accessible to modeling strategies based on electronic structure theory and on derived semi-classical and classical approaches. Therefore, studying elementary processes in nanostructured materials by first-principles simulations provides key information towards understanding – and managing – the sometimes ‘exotic’ aspects of functionalities encountered in everyday applications.

The seminar will briefly introduce intrinsic transport mechanisms in different types of nano materials and outline approaches towards their modeling from a quantum mechanics point of view. Second, the interaction with external triggers such as mechanic or electromagnetic fields and approaches towards the modeling will be introduced. Third, the connection between the functional nanostructure and its embedding environment, e.g. towards electric contacts or with insulating substrate or protection layers is investigated. Examples comprise the electric-field-induced migration of defects in functional oxides [1,2], transport through strain-modified electronic states in semi-conductor nanowires, light-induced conductance changes in single molecules [3], and polarization-modulated tunnel transport in organic thin films [4,5].

References

[1] Hanzig *et al.*, *Phys. Rev. B* **88** (13) 024104.
[2] Seidel *et al.*, *Nat. Mater.* **8** (09) 229.
[3] Sendler *et al.*, *Adv. Sci.* **2** (15) 1500017.
[4] Günther *et al.*, *J. Phys. Chem. C* **120** (16) 9581.
[5] Karpov *et al.*, *Adv. Mater.* **28** (16) 6003.

Host: Robin Santra – CFEL-DESY Theory Division