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## **Multiscale modelling of nanoscale materials and electronic transport**

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To support accelerating materials development cycles we have developed simulation approaches for de-novo characterization and optimization of materials and device properties with nanoscale constituents. A unified multi-disciplinary approach that integrates materials science simulation and high performance computing is required to transform isolated solutions for specific problems into comprehensive, industry-ready platforms, which are capable of predicting the properties of complex materials on the basis of their constitutive elements.

In recent years we have therefore developed simulation methods that describe the conformation and electronic properties of materials built on the basis of well-defined nanoscale constituents. Here we discuss results on single-molecule electronics with application to molecular wires (metallic and organic), on the development of the atomic transistor and organic light emitting diodes.

Die Vortrag findet um **16:15 Uhr** im Gebäude der Materialwissenschaften,  
Lichtwiese, Petersenstr. 23, **Raum 77** statt