Multiscale Modelling with Accelerated Algorithms

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Multiscale Materials Modelling Simulation becomes increasingly important to understand phenomena at the nanoscale and develop novel materials. In recent years, we have developed multiscale simulation approaches for de-novo characterization and optimization of materials and device properties on the basis of their nanoscale constituents. Here we discuss development of the atomic molecular switches [1, 2], the electronic and structural properties of nanocarbon materials [3, 4, 5] and organic semiconductor devices [5, 6]. Small-molecule organic semiconductors are used in a wide spectrum of applications, ranging from organic light emitting diodes to organic photovoltaics. However, the low carrier mobility severely limits their potential, e.g. for large area devices. As an example of our methodology, we present a parameter-free model, which provides an accurate prediction of experimental data over ten orders of magnitude in mobility, and allows for the decomposition of the carrier mobility into molecule-specific quantities. We also demonstrate that a single molecular property, i.e. the dependence of the orbital energy on conformation, is the key factor defining mobility for hole transport materials. The availability of first-principles models to compute key performance characteristics of organic semiconductors may enable in-silico screening of numerous chemical compounds for the development of highly efficient opto-electronic devices.

References

[1] Xie, F.Q., Maul, R., Obermair, C., Wenzel, W., Schon, G. & Schimmel, T. "Multilevel Atomic-Scale Transistors Based on Metallic Quantum Point Contacts." Advanced Materials 22, 2033-+ (2010).

[2] Branchi, B., Karipidou, Z., Sarpasan, M., Knorr, N., Rodin, V., Friederich, P., Neumann, T., Meded, V., Rosselli, S., Nelles, G., Wenzel, W., Rampi, M.A. & Von Wrochem, F. "Self-Assembled Metal-Terpyridine Wires for Robust Large Area Molecular Devices." Adv. Materials (in press) (2016).

[3] Lukas, M., Meded, V., Vijayaraghavan, A., Song, L., Ajayan, P.M., Fink, K., Wenzel, W. & Krupke, R. "Catalytic subsurface etching of nanoscale channels in graphite." Nat Commun 4, 1379 (2013).

[4] Beljakov, I., Meded, V., Symalla, F., Fink, K., Shallcross, S., Ruben, M. & Wenzel, W. "Spin-Crossover and Massive Anisotropy Switching of 5d Transition Metal Atoms on Graphene Nanoflakes." Nano Letters 14, 3364-3368 (2014).

[5] Moench, T., Friederich, P., Holzmueller, F., Rutkowski, B., Benduhn, J., Strunk, T., Koerner, C., Vandewal, K., Czyrska-Filemonowicz, A., Wenzel, W. & Leo, K. "Influence of Meso and Nanoscale Structure on the Properties of Highly Efficient Small Molecule Solar Cells." Advanced Energy Materials 6 (2016).

[6] Friederich, P., Symalla, F., Meded, V., Neumann, T. & Wenzel, W. "Ab-initio Treatment of Disorder Effects in Amorphous Organic Materials: Towards Parameter Free Materials Simulation." Journal of Chemical Theory and Computation (2014).