Very Large Scale Semiempirical MO Calculations on SAM-OFETs

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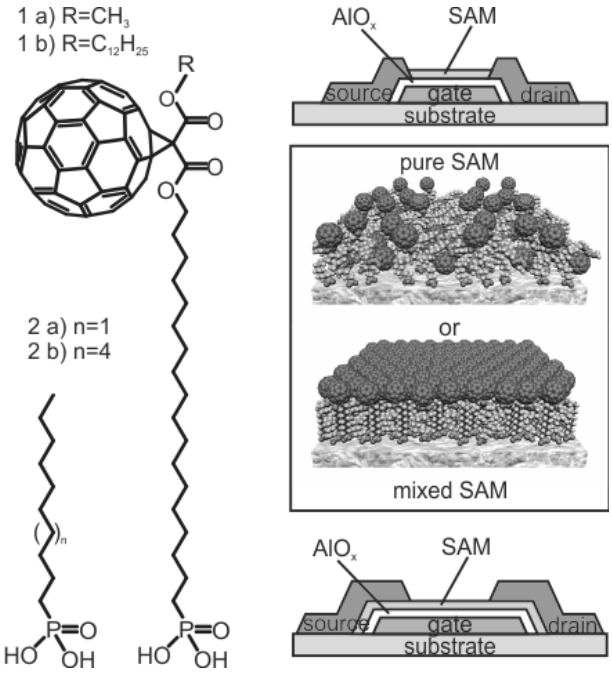
Self-assembled monolayers (SAMs) consisting of mixtures of phosphonic acids **1** and **2** can potentially act as semiconductors in organic field-effect transistors (OFETs).[1] Atomistic molecular-dynamics simulations have been used to study the structural and dynamic properties of these systems.

With our new program EMPIRE, we are now able to look beyond the structural properties and investigate electronic properties by semiempirical molecular orbital (MO) calculations for tens of thousands of atoms.



[1] A. Rumpel, M. Novak, J. Walter, B. Braunschweig, M. Halik, W. Peukert, *Langmuir,* **2011**, *27*, 15016-15023.