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MULTI-SCALE MODELLING OF NANO-SENSORS BASED ON CARBON NANOTUBES (CNTS) AND CONJUGATED POLYMERS FOR WATER QUALITY MONITORING

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We study resistive chemical sensors based on percolating networks of CNTs functionalized non-covalently by conjugated polymers. A change of resistance is expected in water upon complexation of a target ion by a specifically designed polymer probe. Multi-scale modelling aims at understanding and predicting the response of the sensor.

First, we derive the functional dependence of the effective resistance of random percolating networks of stick nanowires on elementary physical parameters (nanowire linear resistance per unit length, nanowire/nanowire contact resistance, metallic electrode/nanowire contact resistance) [1]. This understanding of the three main contributions, of different physical origins, to the whole, experimentally measured sensor resistances, is useful for the design of optimal sensor dimensions and sensible element densities.

Then, we study by means of variable-charge molecular dynamics, based on ReaxFF force field (within LAMMPS), the geometrical features of non-covalent functionalization of CNTs by conjugated polymers [2]. We benchmark the performance of ReaxFF force field for pi-pi stacking interacting compounds against other high-level electronic (DFT) methods, with a focus on the level of theory needed to model accurately London dispersion interactions (wave-function based theory vs. density functional theory) and to capture charge transfer from the organic molecule (or conjugated polymer) to the CNT -- this charge transfer is suspected to act as a doping and to modulate the sensor response.

Finally, we study the complexation of target ions (e.g. chlorine, copper, calcium) by the polymer probes -- designed specifically for their affinity towards given ions -- by means of molecular dynamics simulations in solvent (water) with GROMOS classical force field, within GROMACS code. We test numerically the expected selectivity of the polymer probes to different ions, finding the possible binding sites and their corresponding binding energies. We confirm the binding energies obtained with this classical force field by ab-initio (DFT) calculations -- with CP2K code -- and derive association constants for the different ions and binding sites, with free energy calculation techniques using GROMACS.

References

[1] R. Benda, E. Cancès and B. Lebental, arXiv:1904.04369, to be published in *Journal of Applied Physics*.

[2] R. Benda and al., *in preparation*.

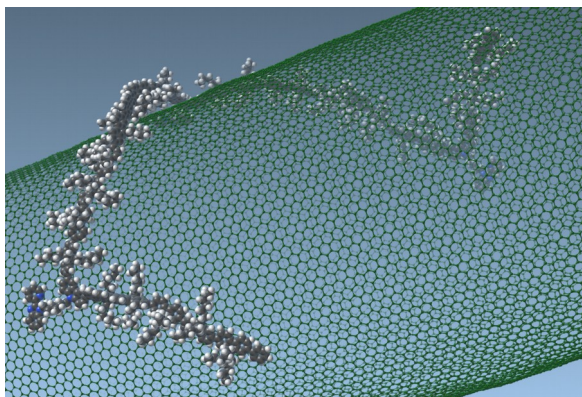


Figure 1 : CNT / conjugated polymer interaction.

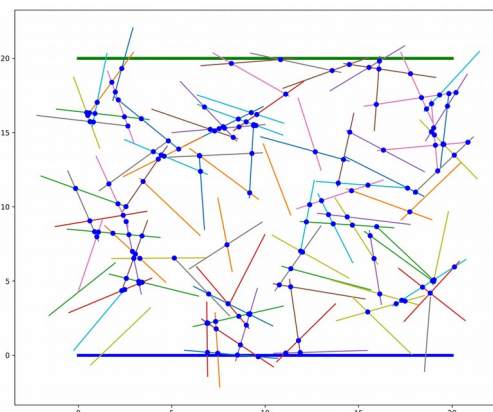


Figure 2: Random 2D percolating network of stick nanowires (e.g. CNTs) whose effective resistance is decomposed into three different contributions.