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Engineering graphene oxide and carbon nanotubes interfaces in bio-systems from first principles to experiments

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The interaction of nanomaterials with biological systems represents today an important research frontier for different applications ranging from regenerative medicine to bio-electronics. For example, the understanding of the interaction mechanisms between nanostructured carbons with proteins of natural origin and/or water can be exploited to investigate new functionalities that can be integrated into functional devices.
Quantum chemistry in this sense has been proven to be of great help to the study of hybrids, in the inorganic, organic, and biological realm [1-5]. Starting from previously reported approaches we here assemble such systems and investigate the role played by functional groups in stabilizing such interfaces, stability which is then experimentally reported to have a major role in the realization of bio-adhesive ink with self-powering properties [1].
Here, we discuss theoretical results of a campaign of *ab-initio* calculations on such heterostructures [1-4], and similarly discuss the observables accessible from first-principles able to support the experimental phenomenon and to shed light on the atomistic mechanism underlying the experimental process. In particular, we report results of a Density Functional Theory based analysis of interfaces between carbon nanotubes with diameter of interest and silk fibroin [1] and between water and graphene oxide [2]. While the former may find applicability in regenerative medicine, the latter is of interest for electrostatic protective composites, i.e. in designing fabrics with antiviral activity.

[1] *S. Bittolo Bon et al., ACS Appl. Mater. Interfaces 13 (2021) 21007–21017.*
*[2] L. Valentini et al. Polymers 12 (**2020**) 1596.*
[3] *L Valentini, et al., Composites Part B: Engineering 166, (2019) 352-360.*
[4] *S. Bittolo Bon et al., Materials & Design, 201 (2021) 109492.*
[5] *Y. Masuda et al., physica status solidi (b) 251 (2014) 1471-1479.*

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