Modelling Alzheimer's Protein Interactions and Electronic Response in Graphene-Oxide Sensors for Early Diagnosis

Damiano Ricciarelli[1]
Viviana Scuderi[1], Rita Turnaturi[2], Gaetano Calogero[1], Simona Filice[1], Simona Crispi[1], Giuseppe Fisicaro[1], Ioannis Deretzis[1], Giuseppina Sabatino[2], Giuseppe Pappalardo[2], Silvia Scalese[1], Antonino La Magna[1]
[1]*Consiglio Nazionale delle Ricerche (CNR), Istituto per la Microelettronica e Microsistemi (IMM), Ottava Strada 5, Catania 95121, Italy.*
[2]*Consiglio Nazionale delle Ricerche (CNR), Istituto di Cristallografia (IC), Via Paolo Gaifami 18, Catania 95126, Italy.*
damiano.ricciarelli@cnr.it

The Alzheimer's disease (AD) is a growing healthcare challenge. [1] Graphene oxide (GO) and its nanostructured derivatives, known for their tunable electro-optical properties, biocompatibility, low toxicity and their ability to interact with complex biological compounds are promising for biomedical sensing applications. [2] In this framework, some of us fabricated a resistive GO-based sensor functionalized with peg4-KLVFF, as schematized in Figure 1(a), to prevent proteins aggregation and enable the selective detection of $A\beta_{42}$, a key AD biomarker. [3] In particular, the sensor exhibits different electrical responses to pathological $A\beta_{42}$ and its scrambled-sequence counterpart, $A\beta_{42s}$.
With machine-learning-based atomistic simulations, where the MACE potential is employed, and protein internal structures are predicted based on amino acid sequences through machine-learning algorithms, [4][5] we reveal key differences in the physisorption, e.g. Figure 1(b)(c), and chemisorption behaviours of $A\beta_{42}$ and $A\beta_{42s}$ respectively. These differences, quantified in terms of interaction energies, explains the sensor's selective electronic response and the impact of its functionalization with peg4-KLVFF on electrical properties. Moving up to density functional theory approaches, we obtain promising results to directly quantify resistivity variations and I-V curves changes occurring in the sensor.

References

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Figures

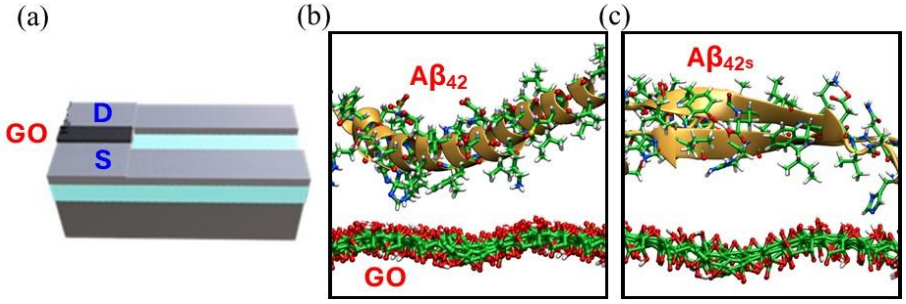

Figure 1: (a) Simplified scheme of the sensor fabricated by some of us, (b)(c) modelled physisorption interaction between proteins and GO.