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ABSTRACT

Interoperable solutions for the simulation of phase change memories

The current and major worldwide drive for big data, machine learning, and quantum computing will push away from traditional all-silicon platforms, and provide a clean slate for industry to rapidly deploy novel technologies based on innovative materials and devices. This requires fast exploration of materials' properties (e.g. memory effects for memristive computing), linking properties to performance in unexplored architectures, and assessing their business potential. Here, we present an interoperable material-to-device simulation scheme for characterization and design of synaptic electronics for neuromorphic computing. This solution is based on the integration of first-principles materials modelling approaches and modelling software for emerging devices, fully compliant with a vision of semantic interoperability, driven by standardized ontologies. In particular, we investigate the switching mechanisms in amorphous $GeTe_4$ glasses, proposed for both volatile and non-volatile memory devices, as a function of dopant insertion. This work is funded by EU NMBP-TO-IND through project INTERSECT, grant 814487.

BIO

Arrigo Calzolari received his PhD in Physics (2003) at *Università di Modena e Reggio Emilia*. He worked as researcher at CNR-IOM Trieste and since 2010 at CNR-NANO Modena. Since Nov. 2012 he is Adjunct Professor Physics Dept., University of North Texas, TX, USA and he had served as External collaborator at Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, IT. AC's scientific activity is focused on the *ab initio* study - within the Density Functional Theory (DFT) framework and beyond (TDDFT, DFPT) - of the structural, optoelectronic, vibrational, plasmonic and transport properties of materials, nanostructures, molecules, and interfaces, for electronic, energy conversion, and nanotechnology applications. Specific themes of research include: complex inorganic materials for electronics and plasmonics; hyperbolic metamaterials; (bio)molecules, polymers and low-dimensional systems, hybrid interfaces for organic electronics and spintronics. Further info at http://amuse.nano.cnr.it.