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Editorial: Methodological and computational developments for modeling the transport of particles within materials

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Editorial on the Research Topic
Methodological and computational developments for modeling the transport of particles within materials

This Research Topic collection deals with the interaction of radiation with matter leading to energy and momentum transfer from the impinging projectiles (be them photons, electrons, or ion beams) to the target material. Depending on the type and the kinetic energy of the primary beam, several processes may occur under irradiation, such as single and collective electronic excitation, ionization of the target atoms, production of an electron cascade that further deposits energy in the sample, and creation of dislocations and vacancies.

Understanding the damage caused by the energy deposition in materials, including those of biological interest, such as DNA, as well as metals and semiconductors, relies on the accurate determination of the chemical-physical mechanisms triggered by the bombardment. This analysis can be carried out by using a variety of methods such as molecular dynamics, Monte Carlo, first principles simulations, and, more recently, artificial intelligence-based techniques. These methodologies differ in both accuracy and computational cost, and their specific use is dependent on the beam as well as the target material. Typically, in classical molecular dynamics electrons are treated implicitly via damping coefficients; in Monte Carlo they follow classical trajectories determined by the elastic and inelastic scattering interactions; conversely, in density functional approaches the Hamiltonian can be made explicitly dependent on ionic and electronic configurations, which makes it possible to model the irreversible transfer of energy into the degrees of freedom of the system, such as the electronic excitation of the atomic constituents also as a function of the charge states of the impinging particles. In this regard, they provide a set of numerical tools able to connect the correlated motion of electrons perturbed by external fields to the macroscale and, notably, to the observables probed in experiments.

In this Research Topic we have collected articles reporting on the methodological developments and applications of state of the art approaches to study the transport of particles within materials, based on *ab initio*, Monte Carlo and machine-learning methods

for simulating the spectral lineshape using different electron spectroscopies and characterisation techniques (XPS, Auger, EELS, REELS, EPES, LEED, SEY . . .).

de Vera et al. used the Mermin Energy Loss Function—Generalized Oscillator Strength (MELF-GOS) approach, based on the dielectric formalism, to calculate charge transport properties of metallic samples, such as the electronic cross sections, stopping power, and energy loss straggling, resulting from the passage of swift protons, alpha particles, and electrons within the solid. Notably, in their analysis, the authors also include the contribution of surface excitations in the low energy regime and propose analytical expressions of the interaction probabilities which can be directly used to compare with experimental data. These calculations are of paramount importance in applications of charged particle beams ranging from the characterisation of materials to hadrontherapy and space technology.

Maille et al. use a similar dielectric approach to assess the secondary electron yields in carbon- and nitrogen-contaminated (and their dioxides) copper surfaces. In particular, the authors calculate from first principles simulations the basic observables, such as the energy loss function, which are used as input in the Monte Carlo approach to investigate electron transport. Furthermore, this work determines the dependence of the secondary electron yield on the Fermi level-to-vacuum potential barrier for the different contaminants.

Werner provides an unified model of the energy-dissipation process of energetic electrons in solids valid for any type of electron beam technique. The author demonstrates the high accuracy of this method by modeling and analyzing several electron spectral lineshapes, obtained from XPS, EPES, and EELS. In particular, the author focuses on the low energy regime, which is recently gaining importance since in this energy range the electrons act both as signal carriers and initiators of electrochemical processes.

Mohebbi et al. use *ab initio* methods based on density functional theory to study the optical and electronic properties of vanadium dioxide to assess the complex dielectric function and its derived quantities, such as the extinction coefficient and refractive index. Their calculations suggest that the combination of PBEsol with HSE functionals provides very accurate outcomes for the optical properties of the VO_2(M) polymorph, delivering the efficient characterization of smart materials for electronic and optoelectronic applications.

Finally, Röding et al. develop a machine learning-based approach to estimate microstructural parameters from SAXS, which is a useful technique for nanoscale structural characterization of materials. They demonstrate that this method delivers both efficiency and accuracy in the simulation of the materials structures and the corresponding SAXS data.

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