Ph.D. in Chemical Sciences
Cycle XXXVI

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Research project title:
Rational design of charge-transport materials for perovskite solar cells

Keywords: Photovoltaics, Transition-metal oxides, Charge transport, Lead halide perovskite, Heterogeneous Interfaces.

Research project abstract:
Perovskite solar cells (PSCs) are a promising technology for highly efficient sunlight harvesting and conversion to electricity at convenient costs. However, few flaws of current devices undermine the PSC long-term stability. Some of them concern the interfaces between the photoactive perovskite and the hole transport layer (HTL), e.g. undesired charge recombination, polarization barriers and oxidation processes. A strategy for solving this problem is to replace the standard organic-based HTL (e.g. Spiro-OMeTAD) with more durable and chemically inert solid-state inorganic materials. Within this framework, this proposal aims at finding new p-type transparent conducting oxides that can be applied as HTL with the most exploited lead halide perovskites. To this end, we will implement a new computational design strategy, based on quantum chemistry, for characterizing the electronic structure features (band alignment, charge transport) and the chemical interactions at the perovskite- HTL interface. The most promising candidate HTL will be tested in experimental PSCs at the ENEA Portici Research Center.