Prof. Michele Pavone is active in the field of computational chemistry since 2004. His PhD thesis in Chemical Sciences (2007, advisor prof. V. Barone) reported the first applications of ab initio MD simulations for theoretical spectroscopy. With a two-year sage as associate research scholar in the group of prof. E. A. Carter at Princeton University (2010-2012) MP shifted his research from molecular spectroscopy to materials sciences, with a specific focus on the design of heterogeneous functional materials for energy conversion and storage. MP now leads a research group with one post-doc and three PhD students, and 5 undergraduate students. He has been National Coordinator of two National Italian grants (PRIN2012 and FIRB 2012) and participated as local PI in two others (PRIN 2009 and PRIN 2015). Currently he is leading the UNINA unit on the computational modeling of electrodes for energy conversion and storage devices within the ENEA-MISE PTR 2019-2021 research program. MP is Vice-Chair and MC member for Italy of the EU-COST project "Computational materials sciences for efficient water splitting with nanocrystals from abundant elements" (CA18234). The main scientific achievements of MP are related to the development and application of effective dispersion-corrected DFT approaches for extended soft materials and for hybrid organic-inorganic interfaces, and the development of the density functional embedding theory. Overall, MP has co-authored more than 90 papers in peer-reviewed scientific journals and have received more than 3900 citations (h-index = 32, source Google Scholar). His scientific activity has been recognized by several awards, the most relevant being the Semerano Prize 2008 (best PhD thesis in Physical Chemistry) and the Roetti Medal 2016 (for best under-40 researcher in Computational Chemistry) by the Società Chimica Italiana, and he has been featured as Emerging Investigator 2017 in the field of materials chemistry for energy by the RSC Journal of Materials Chemistry A.