Abstract: Multiscale models have been very successful in chemistry and biology in order to address and overcome length-scales bottlenecks in the computational characterization of systems composed by components of very different sizes. In particular, continuum models have been longstanding efficient tools to model solvation processes, where a molecular-sized solute, treated with full quantum-mechanical details, interacts with a virtually macroscopic liquid system, modeled as a continuum. Not only the continuum approximation is able to provide results in good agreement with the experiments, but thanks to its much reduced computational cost it allows to include an effective description of environment effects while keeping the high-throughput capabilities of first-principles simulations in vacuum. Here we will show how state-of-the-art continuum solvation models, possibly coupled with other hierarchical atomistic descriptions, can be devised and tuned to address important problems in the field of energy storage and conversion. On one hand, the use of continuum models to describe plasmon-enhanced absorption and emission of molecular pigments in natural light-harvesting proteins will be described, allowing the design of bio-hybrid devices for solar light collection. On the other hand, a recently developed continuum solvation model coupled to first-principles condensed-matter simulation programs will be presented, together with its applications in the characterization of catalytic and electrochemical processes.

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2013 - 2014: Researcher at the Department of Chemistry of the University of Pisa, working on multiscale modelling of plasmon-enhanced bio-hybrid devices and on the simulation of light-harvesting proteins. 
September 2011 - 2012: Postdoctoral associate in the group of Prof. Nicola Marzari at the Institute of Materials of the École Polytechnique Fédérale de Lausanne, developing continuum approaches to study solvation effects in condensed matter and materials science.  
2008 - August 2011: Postdoctoral associate in the group of Prof. Nicola Marzari at the Department of Materials Science and Engineering of the Massachusetts Institute of Technology, USA, working on the in-silico characterisation and design of room-temperature ionic liquids for applications in lithium-ion batteries. 