Núria López' research group focuses on atomistic simulations to understand the mechanisms that govern heterogeneous photo-electro-catalysis. The approaches have been extended to machine learning and analysis of large experimental datasets, as well as contributions to software development and data repositories.

Núria López graduated in Chemistry (1999) and got her Ph.D. degree in Theoretical Chemistry at the University of Barcelona, Spain (1995). She then joined the Center for Atomic-scale Materials Physics led by Prof. Jens K. Nørskov (Denmark Technical University) as a postdoctoral researcher before proceeding to start an independent career at ICIQ from 2005. Prof. López has co-authored over 200 scientific publications and received two grants from the European Research Council (ERC).