Irida-Silicene as promising electrode material for supercapacitors.

A Comparative Study by means of Molecular Dynamics

Hugo X. Rodrigues[1], Isabel A. Silva[2], Luiz Antonio Ribeiro Júnior[1], Marcelo L. P. Júnior[1] and Leonardo J. A. Siqueira[2]
[1]University of Brasília, [2]Federal University of São Paulo

Two-dimensional (2D) materials based on carbon and silicon have received considerable attention as potential electrode candidates for supercapacitors due to their structural and electrochemical properties. In this study, fully atomistic molecular dynamics simulations were performed for four symmetric supercapacitors constructed with Graphene, Irida-Graphene, Silicene, and Irida-Silicene as electrodes. The constant potential model was employed to simulate the electrode polarization under an applied voltage. The silicon-based supercapacitors showed improved performance in terms of power density and energy density when compared with the carbon-based systems. The specific capacitance (F⁄g) obtained for the former is approximately 50 % higher than that of the latter, even though Si atoms are twice as heavy as C atoms. This result is related to the intrinsic roughness of the silicon-based 2D materials, which enhances charge polarization at the electrodes. As a consequence, in addition to the increase in capacitance, a reduction in cell resistance is also observed due to the stronger interaction between the electrolyte counter-ions and the electrode surface. The work further presents a detailed analysis of the electrolyte structuring, providing insights into why silicon-based materials can be considered suitable alternatives for the development of high-performance supercapacitors.