Short Communication

Metal Element Doping Graphene for the Oxygen Electrode: A Density Functional Calculation

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As the fundamental electrochemical reactions, the sluggish kinetics of the oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) limit the commercialization of the renewable fuel cells. Alternative to the commercial precious metal catalysts, the development of inexpensive and efficient dual-functional catalysts is of prominent importance. Herein, based on the density functional theory calculation, the ORR/OER activity of the functional graphene is systematically investigated where the 3d transition metal elements (Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu and Zn) are selected as the doping components, aiming to screen out the efficient candidates for the oxygen electrocatalysis.

Keywords: Oxygen electrode, 3d-TM doped graphene, Fuel cells, DFT

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