Chemical reactivity descriptors evaluation for determining catalytic activity, redox potential, and oxygen binding of metallophthalocyanines

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In this article, we employed density functional theory calculation methods to determine the relationship between the chemical hardness (?), intermolecular chemical hardness (? DA), and nucleophilicity (N) chemical reactivity descriptors, as well as the energy of the occupied frontier orbitals (E a1g), and the electrocatalytic activity of different metallophthalocyanines [MPc's with M=Cr(II), Mn(II), Fe(II), Co(I), Ni(II), and Cu(II)] for the oxygen reduction reaction. Our results suggest that ? DA, N, and E a1g are appropriate parameters to estimate the electrocatalytic activity. On the other hand, the type of the metallic center determines the strength of the oxygen-binding energy, where a strong electronic interaction promotes the efficient electro-reduction of the dioxygen molecule, which is observed experimentally as a high catalytic activity.

Chemical hardness

Intermolecular chemical hardness

Metallophthalocyanines

Nucleophilicity index