

MODELLING DOPED GRAPHENE FOR THE ELECTROCATALYSIS OF THE OXYGEN REDUCTION REACTION (ORR)

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Non-metal doped graphene systems were reported to be excellent electrocatalysts for the ORR and thus potential candidates for an efficient Pt substitution in fuel cells. Among them, boron-doped graphene (**BG**) is considered to be the most promising. [1] In this talk we present our computational study, based on density functional theory (DFT) calculations, of B-doped graphene systems. [2] Firstly, the full oxygen reduction to water is investigated by determining intermediates and transition structures along the various possible reaction pathways on the chemically modified free-standing graphene. Both Langmuir-Hinshelwood and Eley-Rideal mechanisms for the associative and dissociative paths are discussed. Secondly, the effect of an applied potential on this electrochemical reaction is investigated with the methodology by Nørskov and co. [3] in both acidic and alkaline conditions. Finally, the pH effect on the stability of the intermediates of reduction is analyzed in terms of the Pourbaix diagram. In the last part of the talk, we will briefly present a comparative computational/experimental study of the ORR on B-doped and B,N-codoped graphene QD systems. [4]

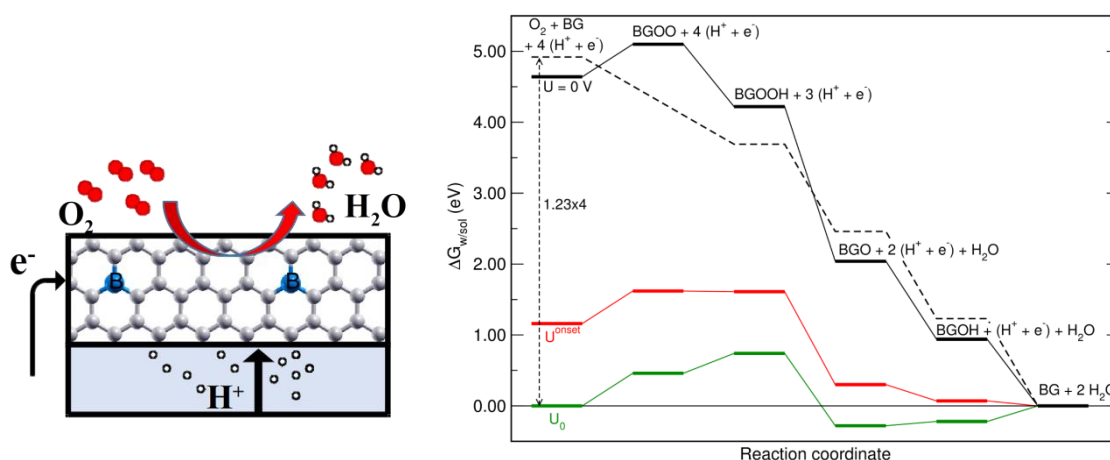


Figure 1: Pictorial representation (left) and free energy diagram (right) of the ORR reaction catalyzed by B-doped graphene in acidic conditions (pH = 0) at different applied potential. Dashed line represents the optimal catalyst.

References

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