A Computational Study of the Synergistic Effect of Ripple and Electric Field on H_2 Dissociation Catalysis in 2D Materials

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Abstract:
As the focus of governments and industries shifts towards sustainability, the demand for sustainable energy sources increases. One such source is hydrogen, which, due to its high energy density and clean burning ability, is used in fuel cells to produce power and for transportation. However, a key limitation associated with this is the use of platinum-based catalysts in the equipment. Platinum is an expensive and scarce precious metal, and it is prone to poisoning, which prevents the widespread adoption of fuel cells.

Viable alternatives that are currently explored to overcome this limitation are 2D materials. Previous studies have shown that introducing ripples, which can occur naturally or due to applied strains, into the structure of graphene enhances its activity as a catalyst for H_2 dissociation [1], [2]. Applying electric fields to the system can also help modulate the electronic structure of these materials and improve the catalytic activity under specific configurations [3]. Despite these individual advancements, there is a lack of research into the combined effect of structural ripples and electric fields in modifying the catalytic performance. In this study, the effect of ripples and electric field is explored on the catalytic activity of a few 2D materials such as graphene, hexagonal boron nitride (hBN), silicene, and gallium nitride (GaN) by Density Functional Theory. Preliminary results on graphene and hBN show that increasing the ripple magnitude decreases the chemisorption energy and dissociation barrier, and specific electric field configurations further enhance the catalytic performance. These findings suggest a synergistic effect between the structural ripples and the electric field that can be leveraged to design efficient, non-precious catalysts for hydrogen-based energy systems. The study is currently being extended to study, in a systematic manner, other 2D materials.

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References

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Figures

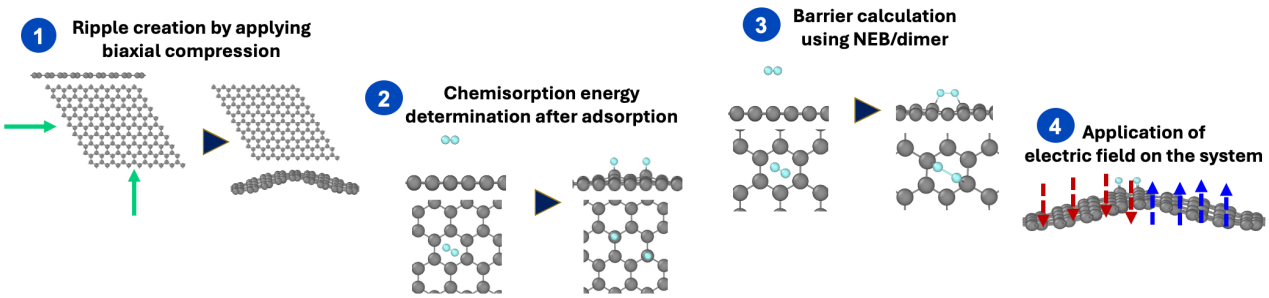

Figure 1: Computational workflow for assessing H_2 dissociation on 2D materials: ripple formation, chemisorption energy calculation, barrier evaluation, and electric field application