

Poulumi Dey  
Assistant Professor



Tel: +31(0)682756809  
E-mail: P.Dey@tudelft.nl  
Website: <http://mse.tudelft.nl>

**Research topics:**  
Ab initio based study of coherent microstructure, Phase stability, Hydrogen embrittlement, Hydrogen storage

## Computation-guided materials designing for H<sub>2</sub> storage applications

### Research activities:

My research focuses on computation-guided design of materials for sustainable and renewable energy application. The demand for energy globally has significantly grown in the past years. Attempts to limit the fossil fuel consumption to prevent the climate change caused by the emissions of greenhouse gases have stimulated the research for alternative, cleaner, sources of energy. In this context, several sources of clean energy e.g., biofuels, solar, hydrogen gas, have been proposed. Hydrogen (H<sub>2</sub>) is one of the most potential candidates for sustainable energy storage that is produced in an eco-friendly manner.

Known bottlenecks in the efficient large-scale realization of H<sub>2</sub>-based technologies is the control over the production, storage and release, as well as the safe transportation of H<sub>2</sub>. To establish a viable 'H<sub>2</sub>-based economy', it is crucial to design materials with properties that allow overcoming these bottlenecks. For instance, the materials for H<sub>2</sub> storage applications should fulfill various requirements such as low weight, robustness (i.e. prevent hydrogen embrittlement), being easily synthesizable and have a low cost. Furthermore, such materials should have rapid adsorption and desorption kinetics in order to act as reversible H<sub>2</sub> storage media. My research interests lie (i) in the identification and optimization of materials for efficient H<sub>2</sub> storage based on multi-scale approach combining quantum mechanical Density Functional Theory (DFT) calculations on phase stability with Molecular Dynamics (MD) simulations on atomistic kinetics (ii) on DFT based materials designing e.g. steels to make them better resistant to Hydrogen Embrittlement (HE).

In a recent work [1], we employed a combined DFT-MD approach to study modifications of graphene at atomistic level for better H<sub>2</sub> storage. The study reveals desorption from defective

hydrogenated graphene structure, V<sub>222</sub>, to be exothermic (Fig. 1). H<sub>2</sub> adsorption-desorption processes are more reversible for V<sub>222</sub> as compared to pristine graphene.

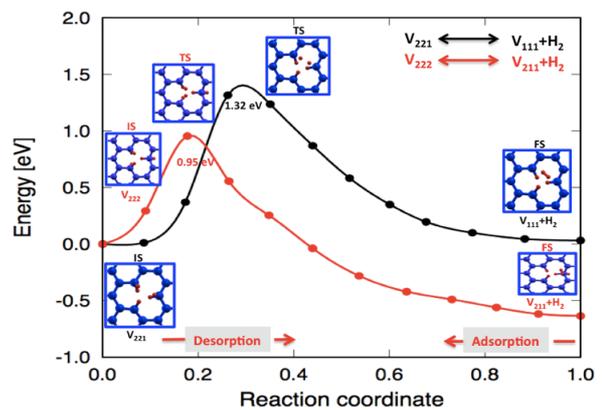


Fig. 1: The red curve is the minimum energy pathway from initial state (IS) V<sub>222</sub> to final state (FS) V<sub>211</sub>+H<sub>2</sub> via the transition state (TS) V<sub>221</sub>. The black curve is minimum energy pathway from IS V<sub>221</sub> to the final state FS V<sub>111</sub>+H<sub>2</sub>. The blue and red atoms represent the C and H atoms, respectively.

Our study shows that V<sub>222</sub> undergoes brittle fracture under tensile loading similar to the case of pristine graphene. The tensile strength of V<sub>222</sub> shows slight reduction with respect to their pristine counterpart, which is attributed to the transition of sp<sup>2</sup> to sp<sup>3</sup>-like hybridization. The study also shows that the V<sub>222</sub> structure is mechanically more stable than the defective graphene structure without chemically adsorbed hydrogen atoms. The current fundamental study, thus, reveals the efficient recovery mechanism of adsorbed hydrogen from V<sub>222</sub> and paves the way for the engineering of structural defects in graphene for H<sub>2</sub> storage.

### Key publications in 2021:

1. G. K. Sunnardianto, G. Bokas, A. Hussein, C. Walters, O. A. Moulτος, P. Dey, *Efficient Hydrogen Storage in Defective Graphene and its Mechanical Stability: A Combined Density Functional Theory and Molecular Dynamics Simulation Study*, International Journal of Hydrogen Energy **46**, 5485 (2021).
2. A. Hussein, A. H. M. Krom, P. Dey, G. K. Sunnardianto, O. A. Moulτος, C. Walters, *The effect of hydrogen content and yield strength on the distribution of hydrogen in steel: a diffusion coupled micromechanical FEM*, Acta Materialia **209**, 116799 (2021).