
Influence of the van der Waals interactions in the chemisorption of N₂ on W(100)

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Résumé

The dissociative adsorption of N₂ on W(100) is theoretically investigated by means of quasi-classical trajectory simulations making use of a density functional theory-based potential energy surface constructed using the vdW-DF2 functional. In this work, the resulting quasi-classical dynamics calculations are compared to those obtained using the PES built with the PW91 functional as well as to the available experimental data. An overall similar topology is found for both potential energy surfaces, however, including the van der Waals functional causes changes in the height of the potential barriers and the deepness of the wells observed before, leading to a different behaviour of the dynamics. A qualitative agreement with experiments is found for the first time for the chemisorption studied.

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