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Catalytic role of defective carbon substrates in the dissociation of small molecules MILEN KOSTOV, Chemical Engineering, North Carolina State University, AARON GEORGE, Physics, NCSU, ERIK SANTISO, KEITH GUBBINS, Chemical Engineering, NCSU, MARCO BUONGIORNO NARDELLI, CHIPS & Physics, NCSU; CCS-CSM, Oak Ridge National — A necessary step towards the achievement of a hydrogen economy is the development of a production process that is able to drastically revamp the energetic cost while leaving, at the same time, a smaller environmental footprint than the current industry standards. Chemical reactions are often carried out in nano-structured media, where the reaction mechanism can be dramatically changed due to the interactions of reacting species with the substrate. One point of interest is the recent experimental evidence for stable defects in graphene layers such as vacancies. Our aim is to report that physical and chemical properties of such defects can have an astounding effect on certain chemical reactions. Using state of the art first principles modeling techniques, we have explored the potential of nano-structured carbon materials to lower the activation energy barrier of dissociation reactions for small molecules. Using water as a prototypical example, we will show how the carbonaceous environment and the defects present in it, can aid in lowering the activation energy barrier of adsorption and dissociation reactions. Finally we will discuss this exploration in the context of a complete cycle of energy storage and release through the production of hydrogen in defective carbon substrates.

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