Water-driven oxidation of single-layer graphene under strain

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Density functional theory calculations for the oxidation of water on strained and unstrained single-layer graphene were used to investigate tuning chemical reactivity of graphene (e.g. transverse, longitudinal, and biaxial strain). Furthermore, vacancy effect was considered for the change of chemical properties of defect site under strain. First, water oxidation reaction was predicted based on the orbital structure calculation. And the electron density profile on graphene sheet and binding energy between graphene and functional groups were calculated as an evidence for the change in reactivity with increasing strain. Finally, we calculated the Gibbs free energy at each step for water oxidation reaction with different directions of strain. We found that strain enhances the chemical reactivity on defective graphene surface.