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Graphenic C_3N_4: A New Template for Metal Decoration and Hydrogen Adsorption[1] YI ZHANG, University of Nevada, Las Vegas, HONG SUN, Shanghai Jiao Tong University, China, CHANGFENG CHEN, University of Nevada, Las Vegas — From density functional theory calculations we identify a graphenic C_3N_4 (g-C_3N_4) structure as an excellent template for stable and well dispersed decoration of alkali and transition metal atoms which, in turn, exhibits a high capacity for hydrogen adsorption with binding energies (a few tenths of eV) suitable for mobile applications. The unique porous micro-structural sites of g- C_3N_4 accommodate the excessive N lone-pair electrons and promote strong hybridization between the orbitals of N and metal atoms. It plays a key role in overcoming the tendency of metal-atom clustering that has plagued other proposed hydrogen storage media. These metal decorated g- C_3N_4 may also prove useful in a variety of catalytic and sensing applications.

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