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Exploiting Nano-geometrical effects in Energy: Storing hydrogen, adsorbing light, catalyzing reactions

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Nanoscale geometries provide several novel mechanisms towards modifying materials properties for energy applications. In particular, I will discuss the theory of how geometrical constraints on atomic positions can be used to stabilize dispersions of atoms across surfaces in thermodynamically stable states - a configuration at odds with atoms' natural tendency to aggregate. The first such mechanism is divides space into two disconnected zones separated by an impenetrable suspended graphenic sheet with adsorption of otherwise highly co-reactive species, such as alkali and halogen, in opposite subspaces. These systems could find application in broadly tunable bandgap systems, catalysts for energy applications, and new correlated states of matter. The second mechanism involves creating a profound electron deficiency in an sp^2- bonded carbon layer, and then saturating this deficiency through atomically dispersed metals. These dispersed atoms could then provide a novel substrate for hydrogen storage.