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Hydrogen Storage in Ti Doped Nano Porous Graphene[1] SA LI, PURU JENA, Virginia Commonwealth University, DEAPARTMENT OF PHYSICS, VIRGINIA COMMONWEALTH UNIVERSITY TEAM — Clustering of Ti on carbon nanostructures has proved to be an obstacle in their use as hydrogen storage materials. Using density functional theory we show that Ti atoms will not cluster when doped into nanoporous graphene. With each Ti atom binding up to four hydrogen molecules with an average binding energy of 0.54 eV/H2, this material can be ideal for storing hydrogen. Equally important, nanoporous graphene is magnetic with or without Ti doping, but magnetism disappears when fully saturated with hydrogen. This novel feature suggests that nanoporous graphene can also be used as a hydrogen sensor.

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