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Hydrogen storage of calcium atoms adsorbed on graphene: First-principles plane wave calculations CAN ATACA, ETHEM AKTURK, SALIM CIRACI — Based on the first-principles plane wave calculations, we showed that Ca adsorbed on graphene can serve as a high-capacity hydrogen storage medium, which can be recycled by operations at room temperature. Ca is chemisorbed by donating part of its 4s-charge to the empty π^*-band of graphene. At the end adsorbed Ca atom becomes positively charged and the semi-metallic graphene change into a metallic state. While each of adsorbed Ca atoms forming the (4×4) pattern on the graphene can absorb up to five H_2 molecules, hydrogen storage capacity can be increased to 8.4 wt % by adsorbing Ca to both sides of graphene and by increasing the coverage to form the (2×2) pattern. Clustering of Ca atoms is hindered by the repulsive Coulomb interaction between charged Ca atoms.

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