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Title: Effect of adatoms and molecules on the physical properties of Platinum-doped and -substituted silicene: A First-Principles Investigation

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- 1. Silicene has a small band gap by Pt adsorption or turn into metallic system by Pt substitution.
- 2. Oxygen adsorbed Pt/silicene system is a half-metallic ferromagnet with 1.48 μ_B magnetic moment.
- 3. Pt-embedded silicene systems are narrow gap semiconductors upon adsorption of CO, CO2, and CH4 molecules.
- 4. C, H, and O atoms bind on Pt-embedded silicene with large adsorption energies.
- 5. Eley-Rideal mechanism is convenient to form CO2 molecule from CO and O2 for Pt substituted silicene.

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