Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Stanene Based Gas Sensors: Effect of Spin-Orbit Coupling

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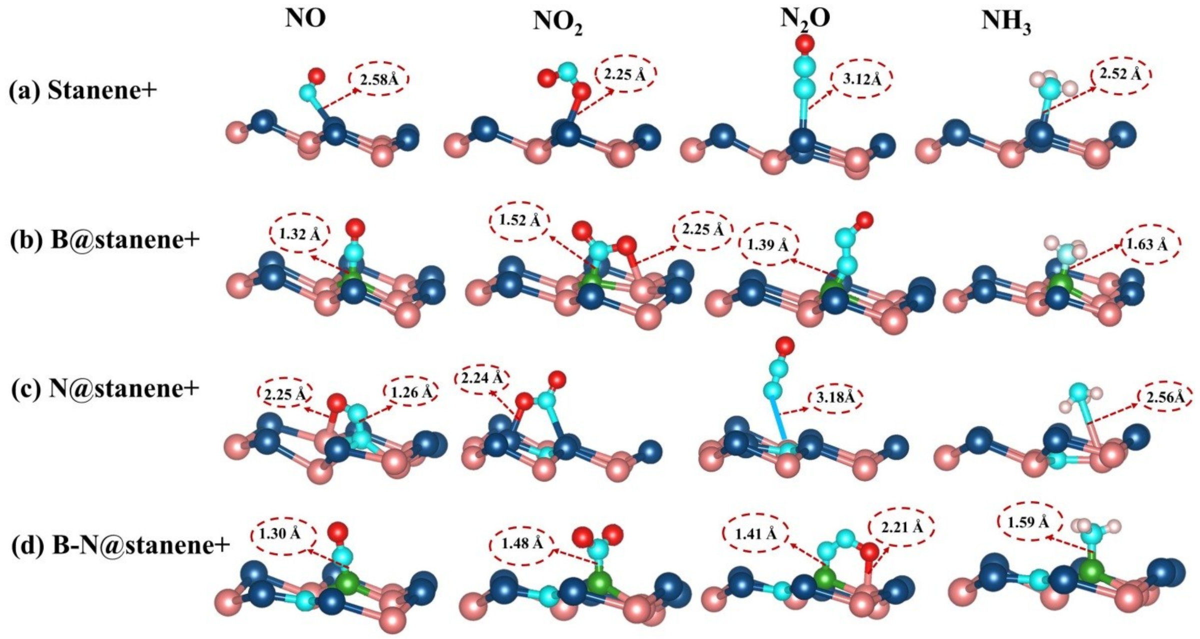
Text S1: Brief description of spin orbit coupling (SOC)



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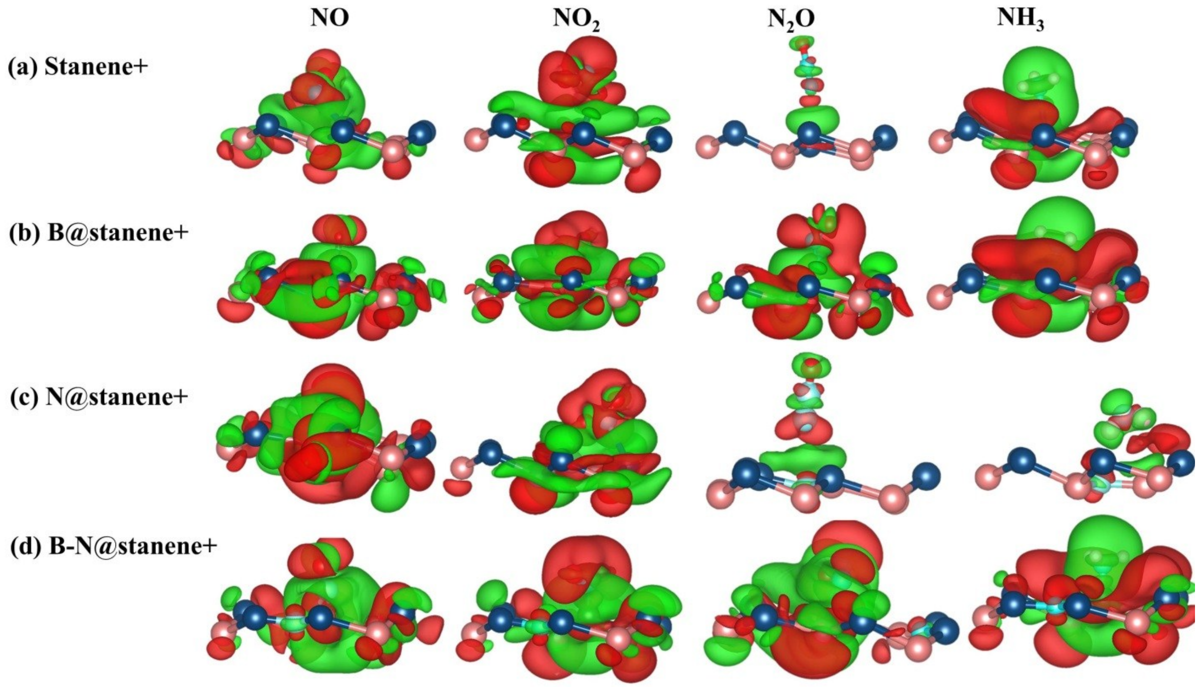

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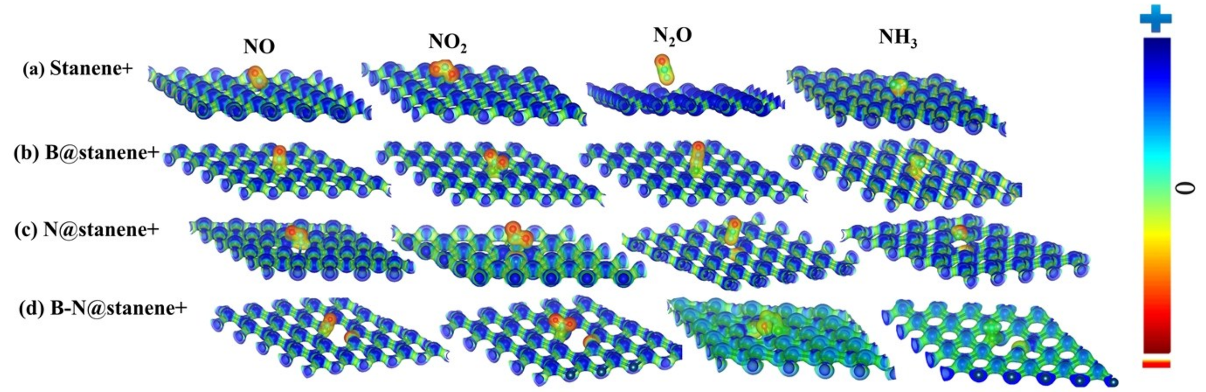
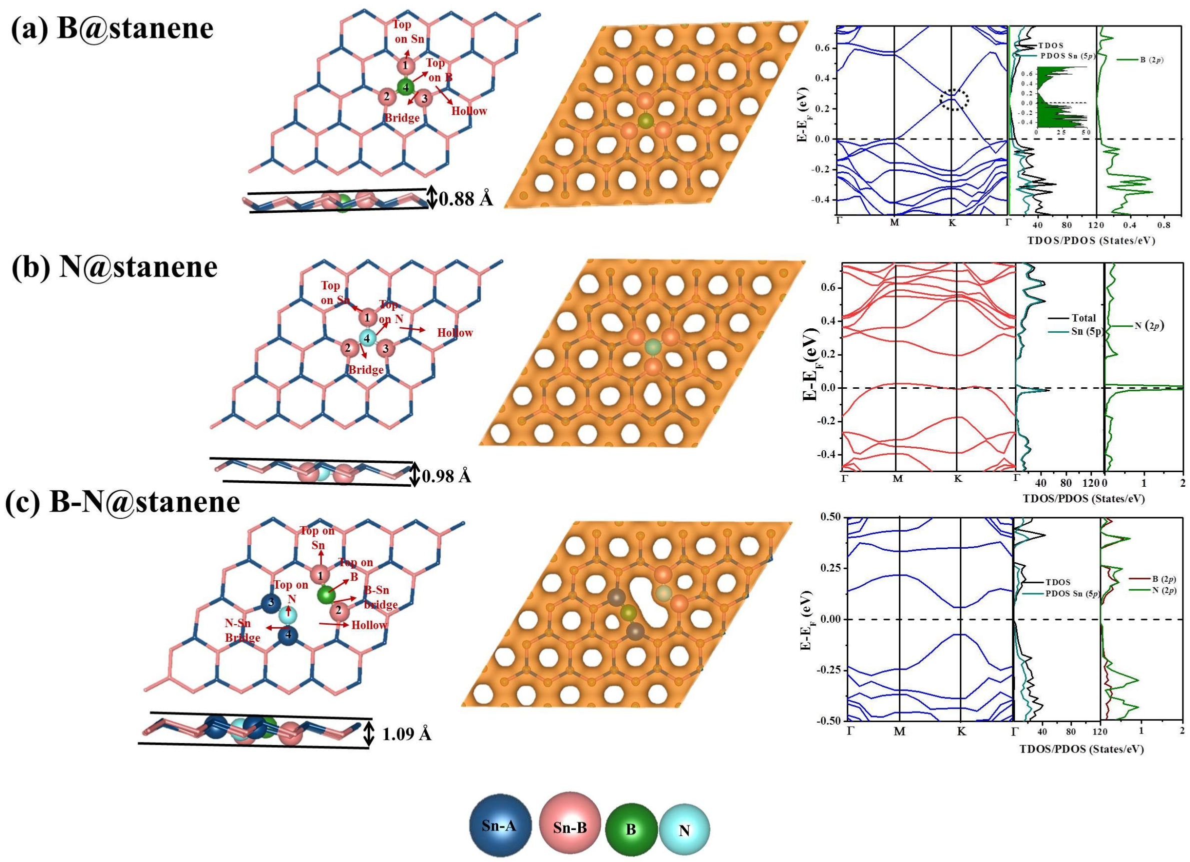


Figure S3: Electrostatic Potential (ESP) surface plots of (a) NO, (b) NO$_2$, (c) N$_2$O and (d) NH$_3$ adsorbed pure and doped (B@-, N@-, and B-N@) stanene. Isosurface value is 0.031 e. Å^{-3}.



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Text S1: Brief description of spin-orbit coupling (SOC)

The spin-orbit coupling (SOC) is a relativistic effect, which is responsible for splitting electronic bands. In this phenomenon, electron's spin and the magnetic field generated by the electron's orbit around the nucleus shows electromagnetic interaction, which splits the energy levels. The effect is significant for heavy elements due to relativistic effect.[1] Thus stanene shows large SOC effect compared to graphene, silicene and germanene.[2] For a two-dimensional sheet of electrons in the x-y plane, the simplest Hamiltonian is

$$\hat{\mathrm{H}}_{SO} = -\frac{\alpha}{\hbar}\lfloor \rho \times \sigma \rfloor_z$$

where the index z denotes the z component of the operator in the vector $\lfloor \rho \times \sigma \rfloor$ product and α is the Rashba parameter. By applying additional `back-gate' voltages to the structure the Rashba parameter α can be changed externally. Thus, the change in α can be used to manipulate electron spins due to change in the spin-orbit coupling.

Reference

1. A. Kuc, and T. Heine, *Chem. Soc. Rev.,* 2015, **44,** 2603-2614.
2. Y. Xu, B. Yan, H-J. Zhang, J. Wang, G. Xu, P. Tang, W. Duan, S-C. Zhang, *Phys.Rev. Lett.,* 2013, **111,** 136804.