

## SUPPORTING INFORMATION

# Explosive Molecule Sensing at Lattice Defect Sites in Metallic Carbon Nanotubes

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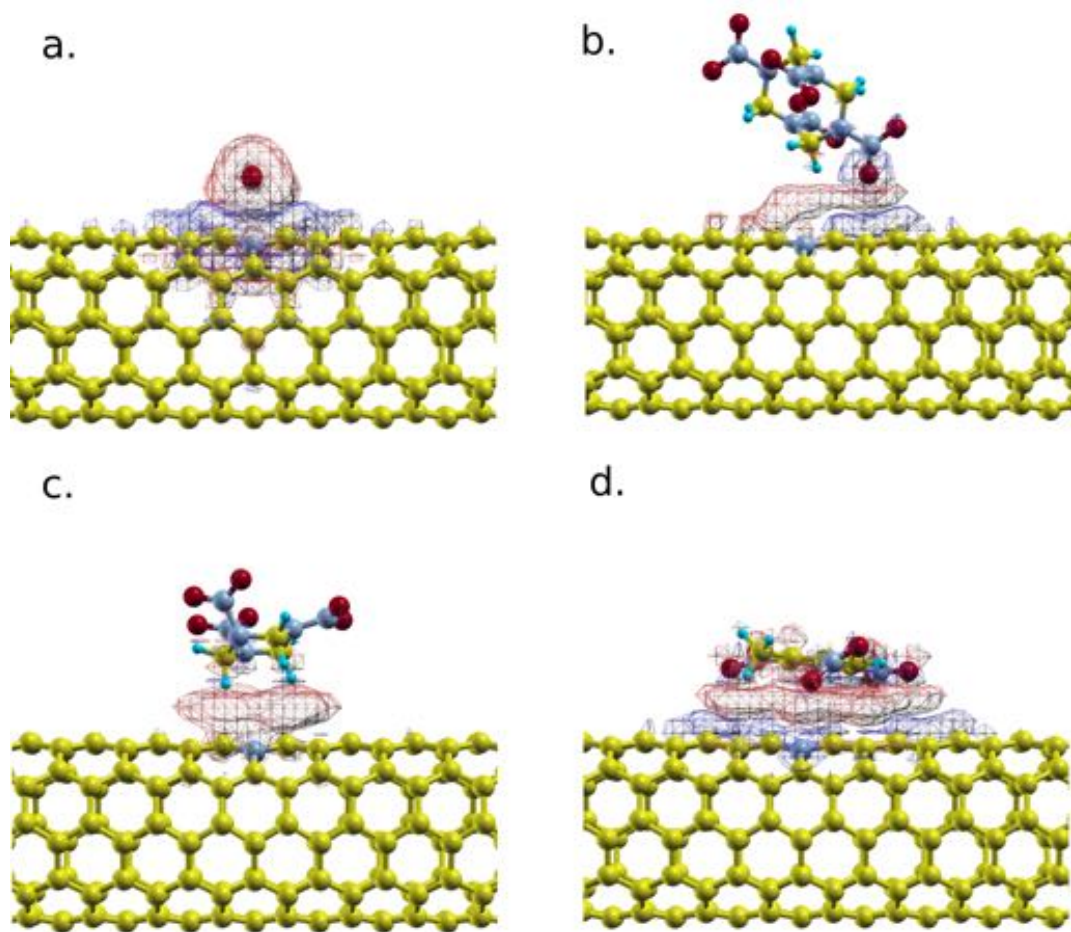


Figure S1: Charge density difference plots for sensing by a nitrogen-doped CNT(5,5): (a) O<sub>2</sub> sensing, (b) HMX sensing, (c) RDX sensing, and (d) TNT sensing

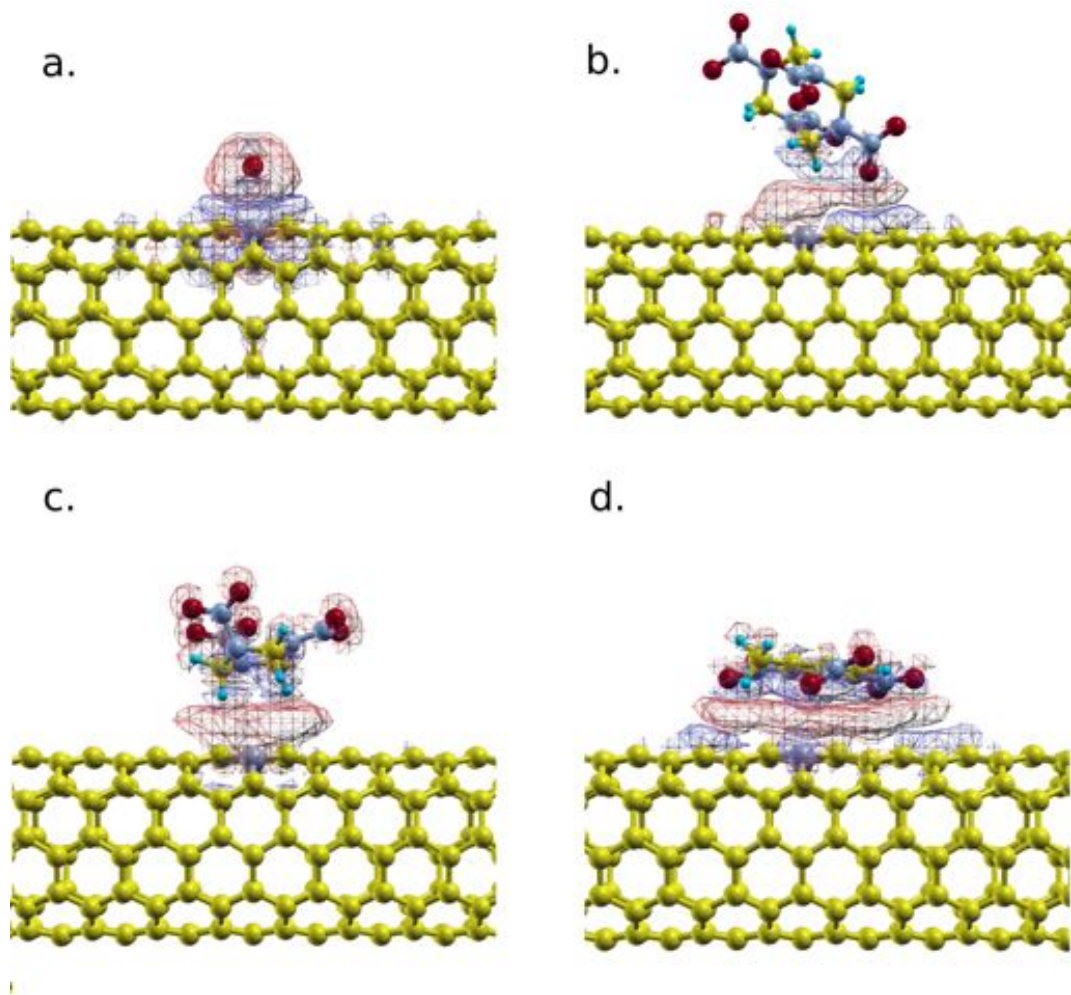


Figure S2: Charge density difference plots for sensing by a boron-doped CNT(5,5): (a) O<sub>2</sub> sensing, (b) HMX sensing, (c) RDX sensing, and (d) TNT sensing

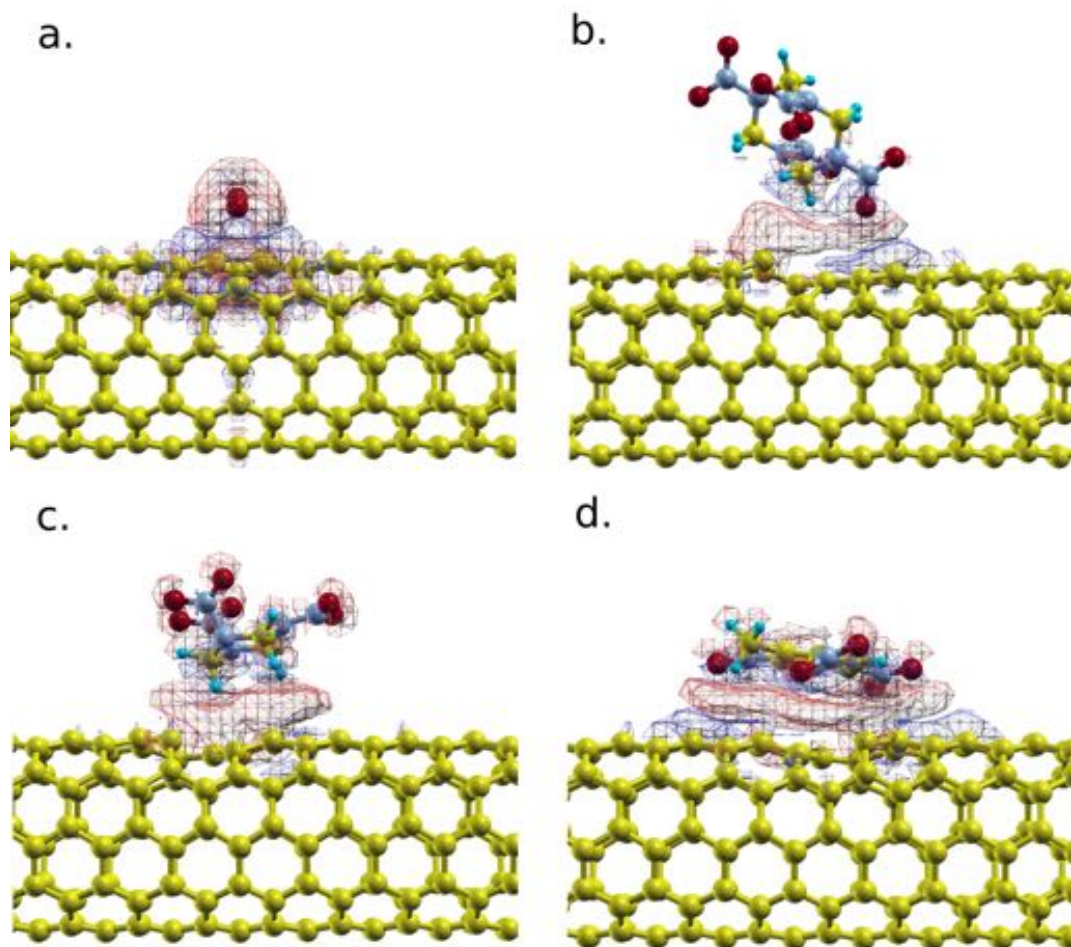


Figure S3: Charge density difference plots for sensing by a CNT(5,5) with a vacancy defect: (a) O<sub>2</sub> sensing, (b) HMX sensing, (c) RDX sensing, and (d) TNT sensing

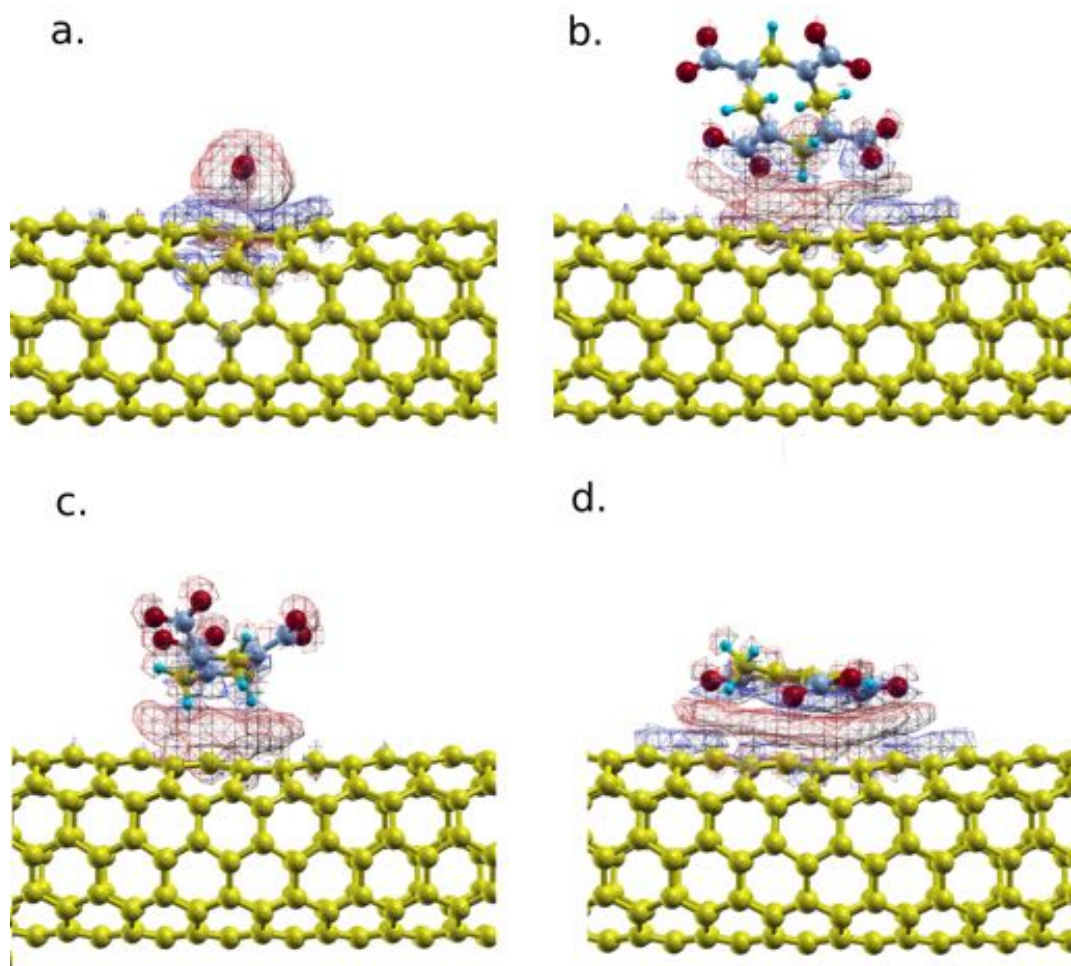


Figure S4: Charge density difference plots for sensing by a CNT(5,5) with a divacancy defect: (a) O<sub>2</sub> sensing, (b) HMX sensing, (c) RDX sensing, and (d) TNT sensing



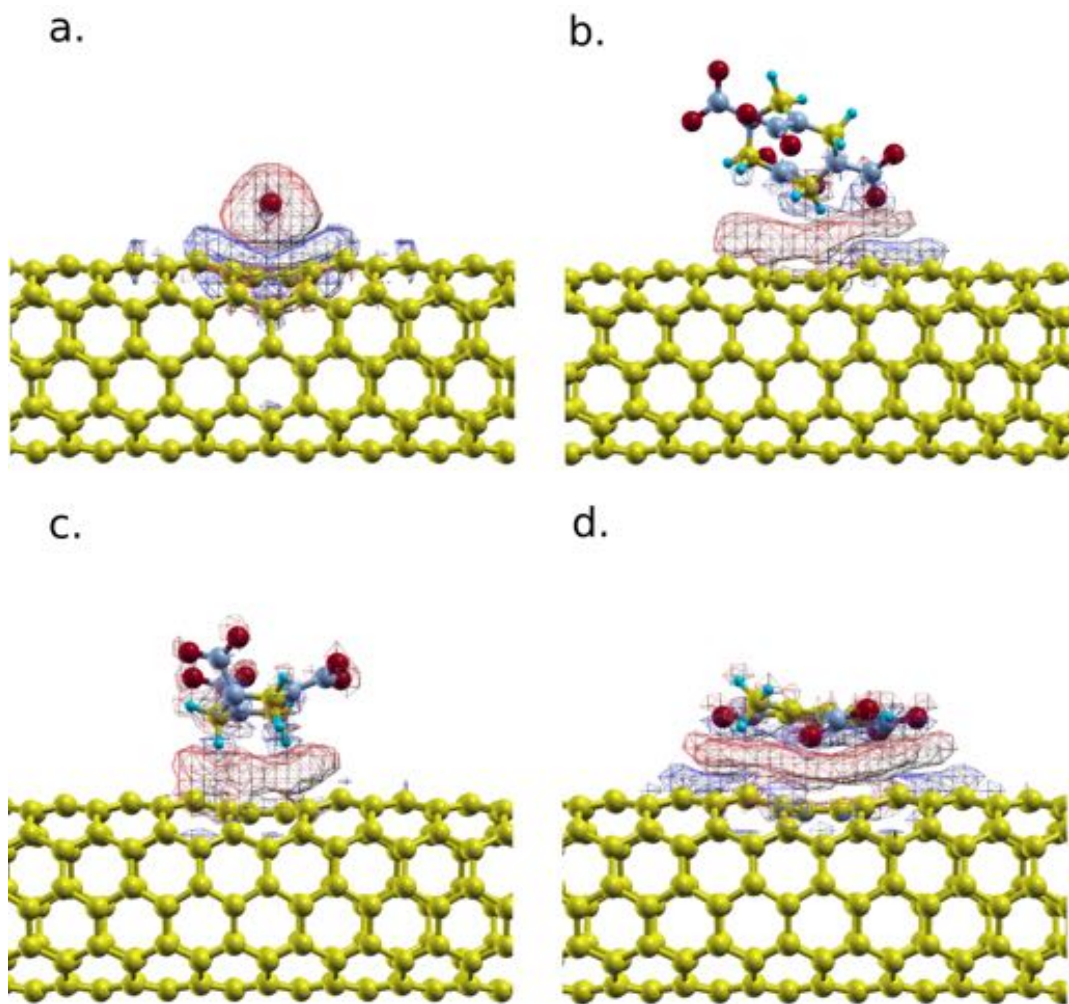


Figure S5: Charge density difference plots for sensing by a CNT(5,5) with a Stone-Wales defect: (a) O<sub>2</sub> sensing, (b) HMX sensing, (c) RDX sensing, and (d) TNT sensing