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

Understanding the first half-ALD cycle of the ZnO growth on hydroxyl functionalized carbon nanotubes: Supplementary section

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Analysis of forces

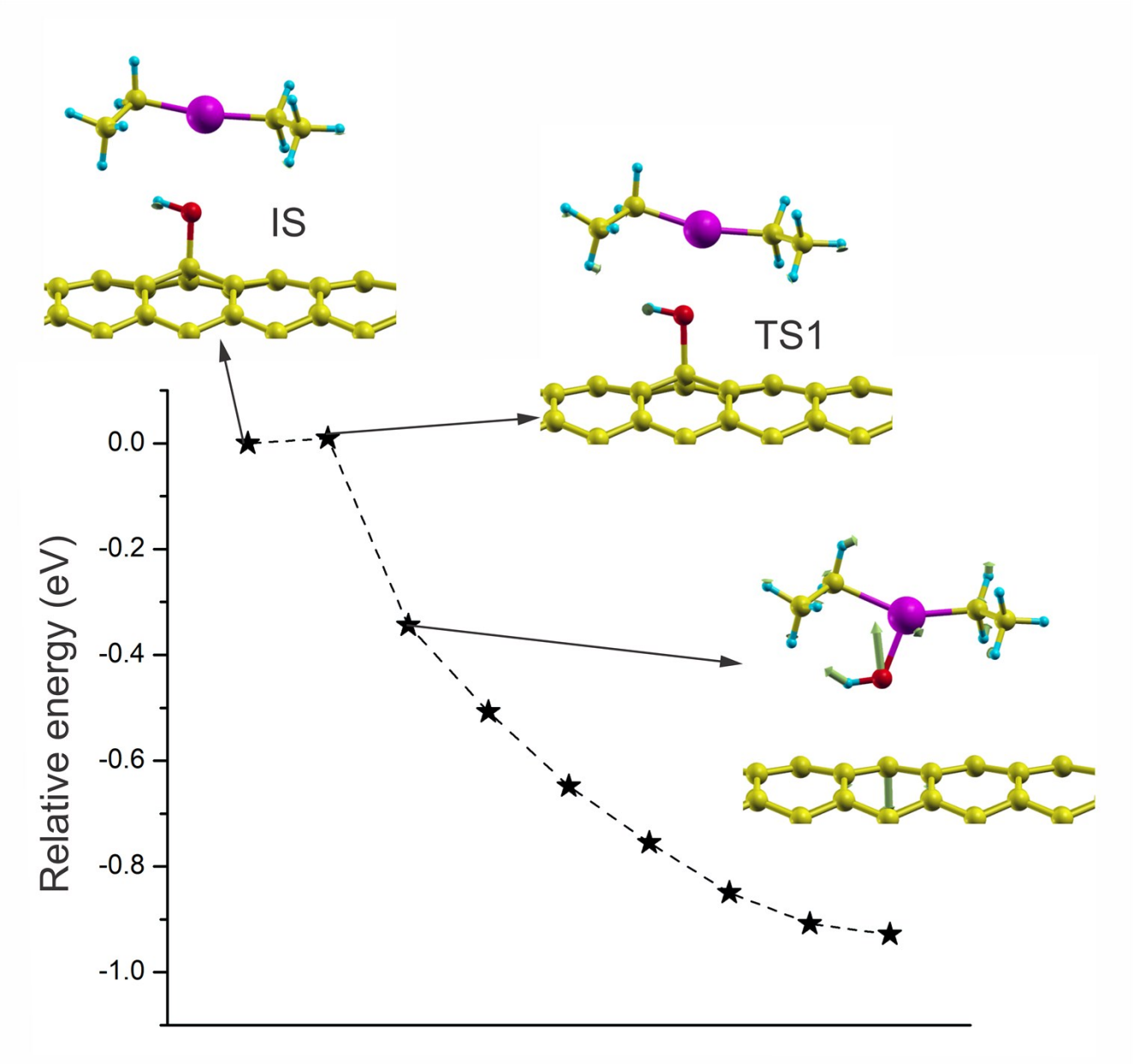

Figure S1a. Projection of forces on the main states of the reaction from IS to 2S.

Minimum energy pathway from IS to 2S. By definition the IS is a minimum, while the TS1 is a saddle point. Both show zero forces (forces are depicted as yellow arrows in each atom). On the other hand, the third point in the pathway is indeed an instable point, with forces different from zero.

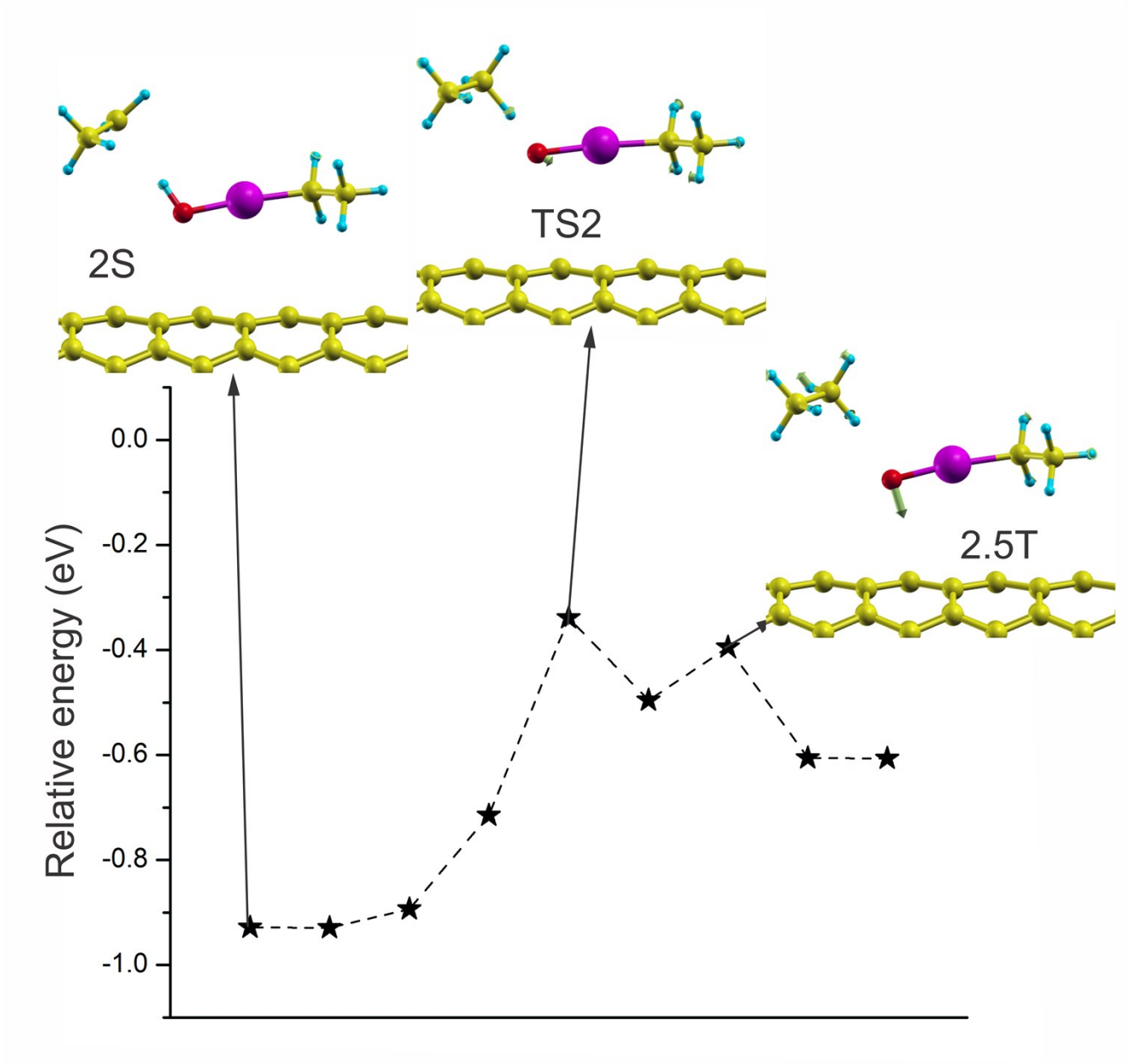

Figure S1b. Projection of forces on the main states of the reaction from 2S to 3S.

Minimum energy pathways from 2S to 3S states. As in the previous path, 2S depicts a zero force in all atoms, meaning that it is a stable minimum point. TS2 state is a saddle point, with zero forces in all atoms. 2.5T state on the other hand, has non-zero forces mainly in the Oxygen atom, which means that the state is not a transition state.

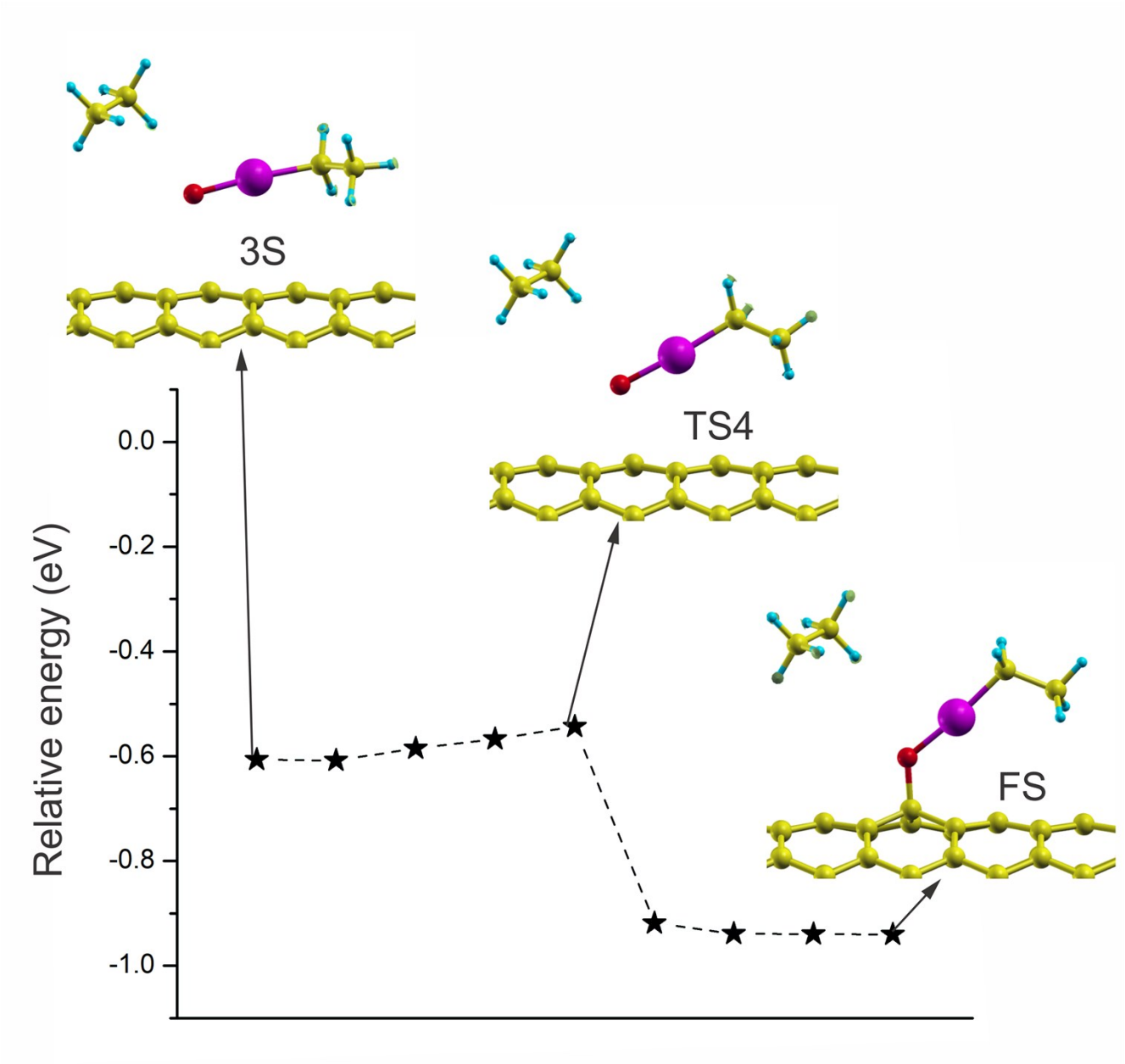

Figure S1c. Projection of forces on the main states of the reaction from 3S to FS. There is a clear transition state (TS4) and 2 stable equilibrium points (3S and FS states), as consequence the unstable equilibrium has a negative second derivative whereas the stable equilibrium points have positive second derivatives.

From the previous force analysis, we have demonstrated that IS, 2S, 3S, FS, and TS1, TS2, TS4 are local minima, and saddle points, respectively. In the saddle points, the second derivative is negative, while in the stable minima points the second derivatives are positive.

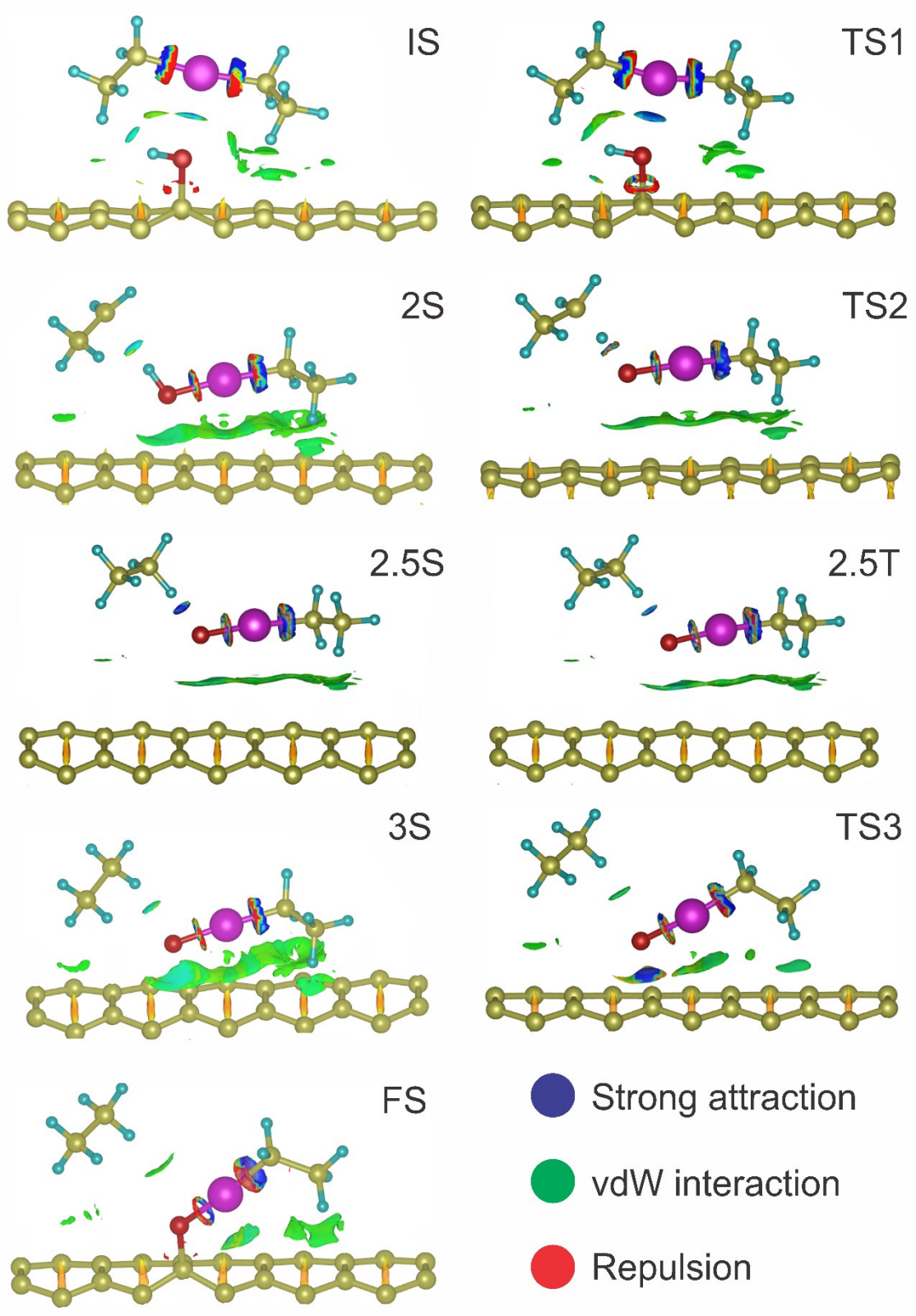

Figure S2. Full non-covalent index analysis. The interaction strength is determined through the second eigenvalue of the density Hessian: Red (positive) denotes steric repulsion, Blue (negative) accounts for attraction (H bridges, etc.), and Green displays weak van der Waals interactions (values ~0).

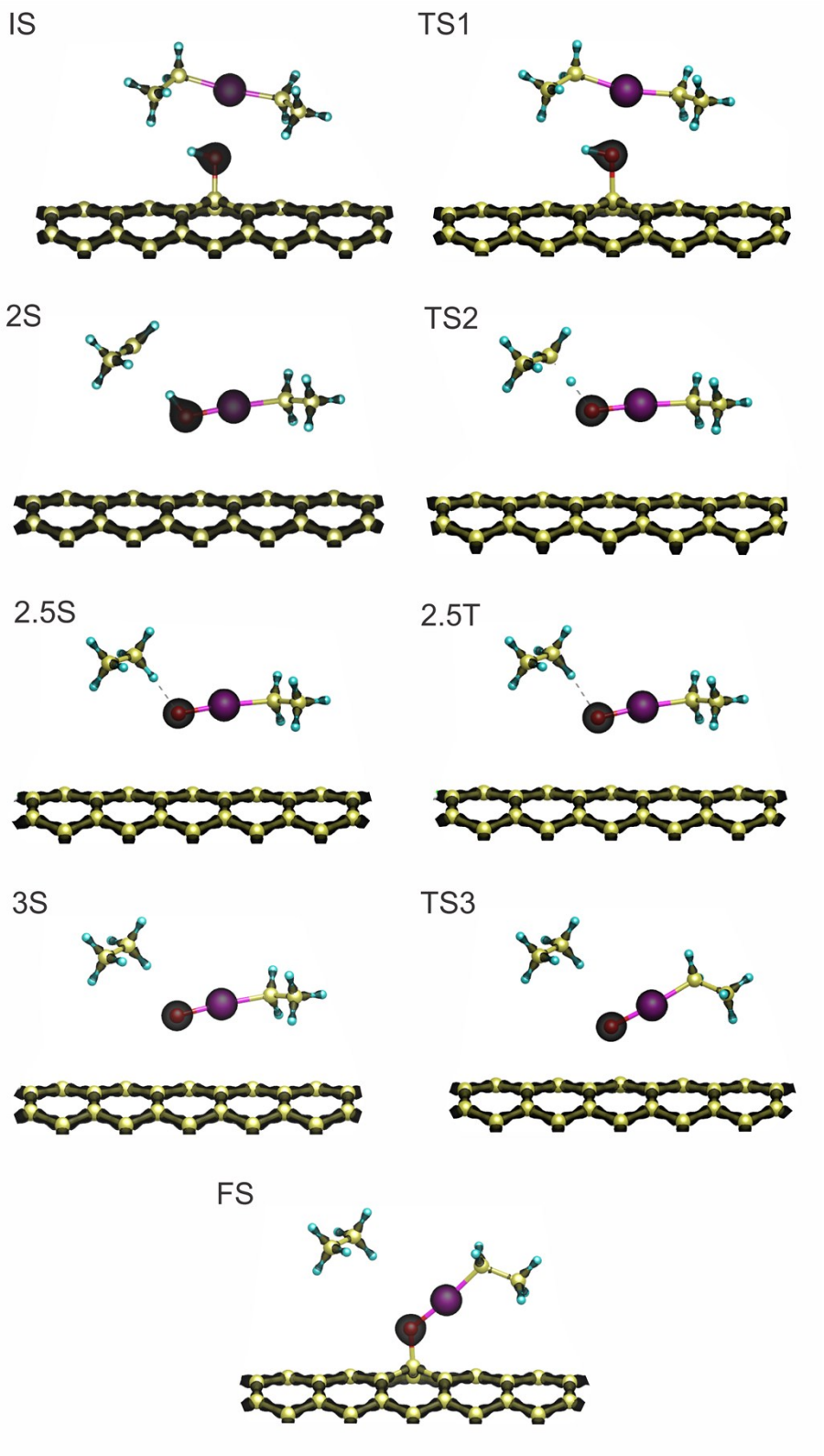

Figure S3. Charge density distributions showing C-C covalent bonds, and characteristic charge densities at Zn and O atoms. (isovalue ρ=0.3).