Mechanisms of Formaldehyde and C_2 Formation from Methylene Reacting with CO_2 Adsorbed on Ni(110)

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Supporting Information

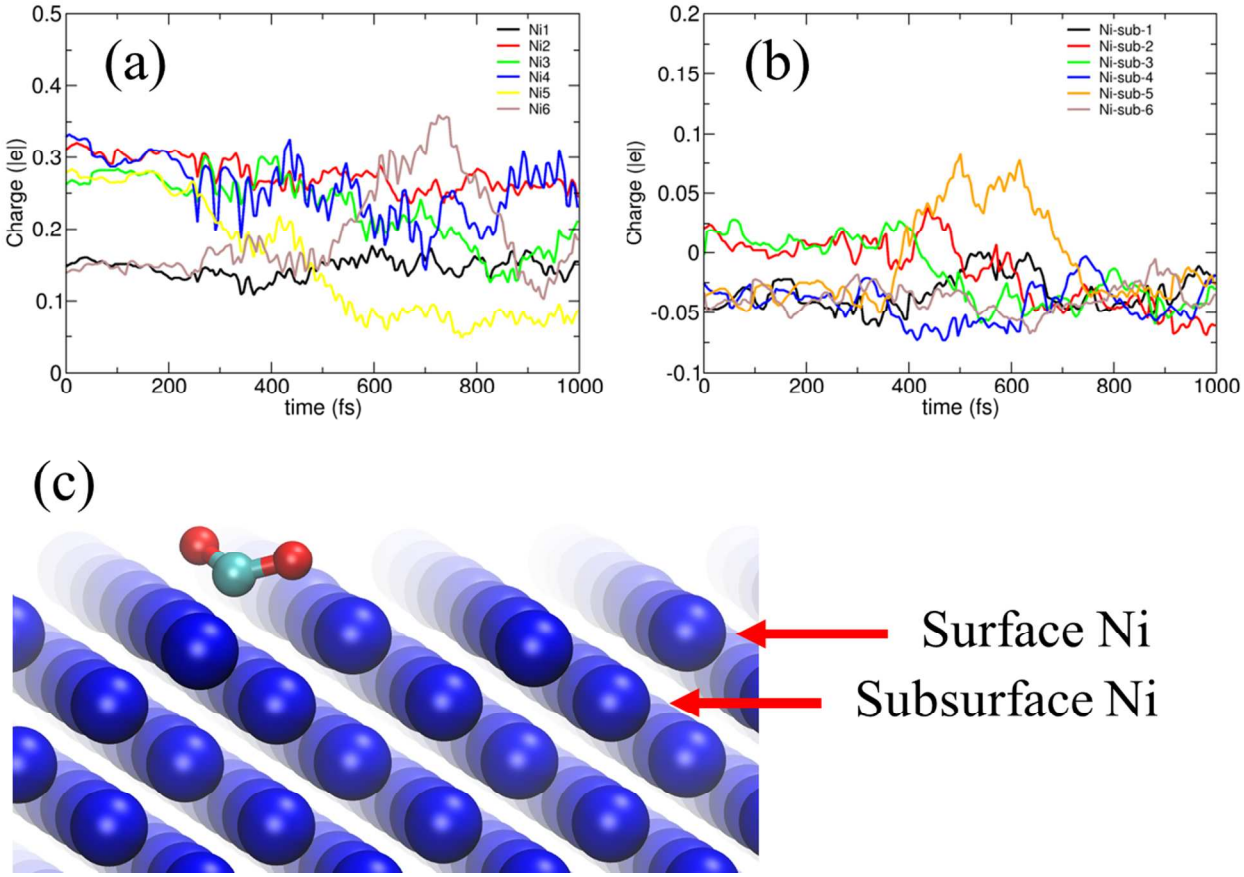

Figure S1. Atomic Bader charges of **(a) surface and (b) subsurface Ni** for a trajectory which corresponds to the **$CH_2 + CO_2^* \rightarrow H_2CO^* + CO^*$** reaction. (c) Definition of the surface and subsurface Ni.

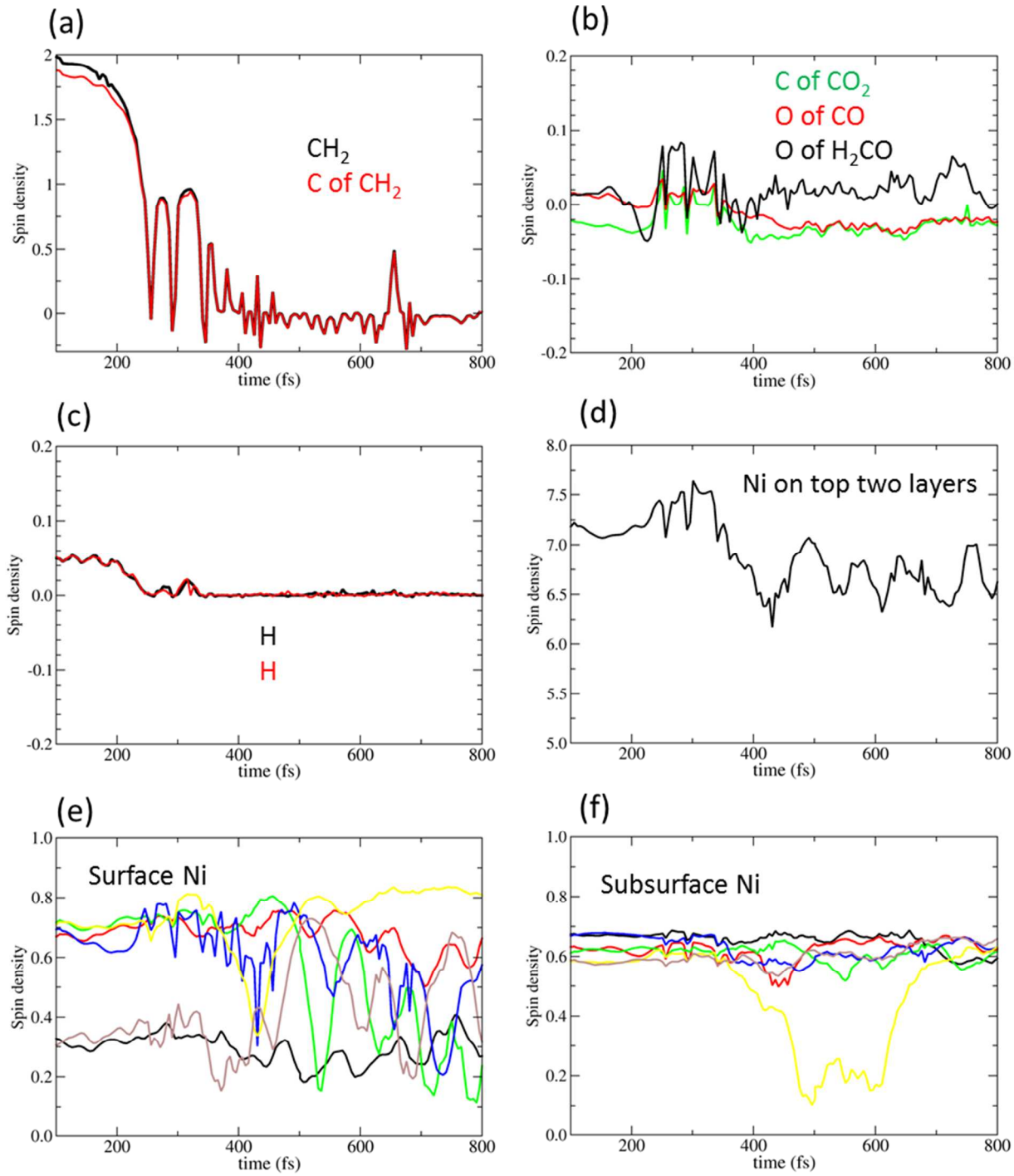

Figure S2. Evolution of spin densities for a trajectory which corresponds to the **CH_2 + CO_2* → H_2CO* + CO*** (Reaction 1 in Section 3.2 of the manuscript). Spin densities of (a) CH_2 and carbon in CH_2; (b) carbon of CO_2 and two oxygen atoms; (c) hydrogen atoms; (d) Ni on top two layers; (e) six surface Ni atoms; and (f) six subsurface Ni atoms.

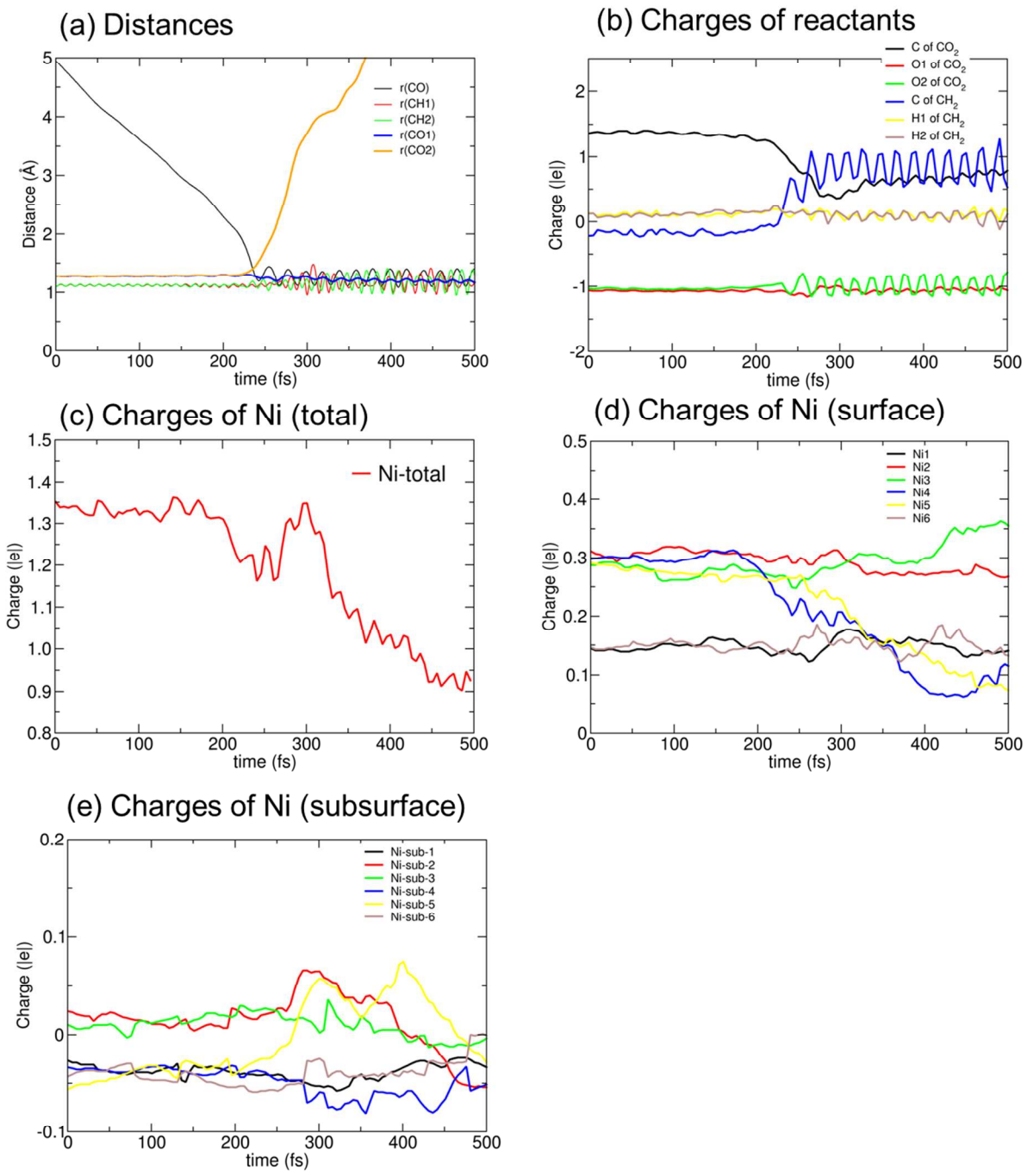

Figure S3. (a) Bond distances and atomic Bader charges of (b) reactants, (c) total Ni atoms, (d) surface Ni atoms, and (e) subsurface Ni atoms for a trajectory which corresponds to the **CH_2 + CO_2* → H_2CO (gas) + CO*** with ER mechanism.

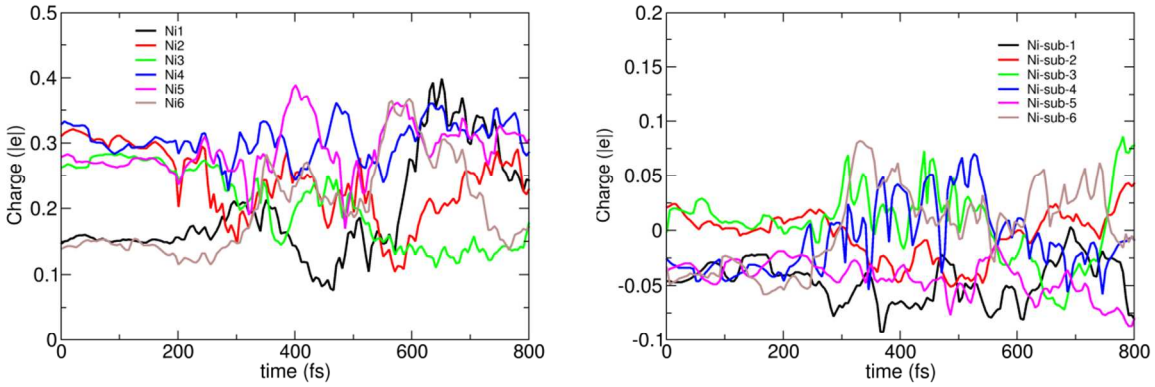

Figure S4. Atomic Bader charges of **surface (left) and subsurface (right) Ni** for a trajectory which corresponds to the $\mathbf{CH_2 + CO_2^* \rightarrow 2H^* + 2CO^*}$ reaction.

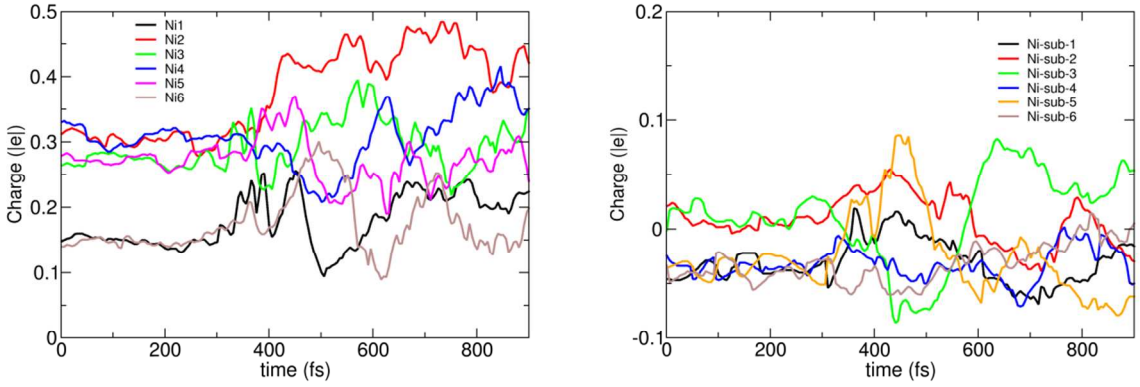

Figure S5. Atomic Bader charges of **surface (left) and subsurface (right) Ni** for a trajectory which corresponds to the $\mathbf{CH_2 + CO_2^* \rightarrow H_2C\text{-}CO_2^*}$ reaction.

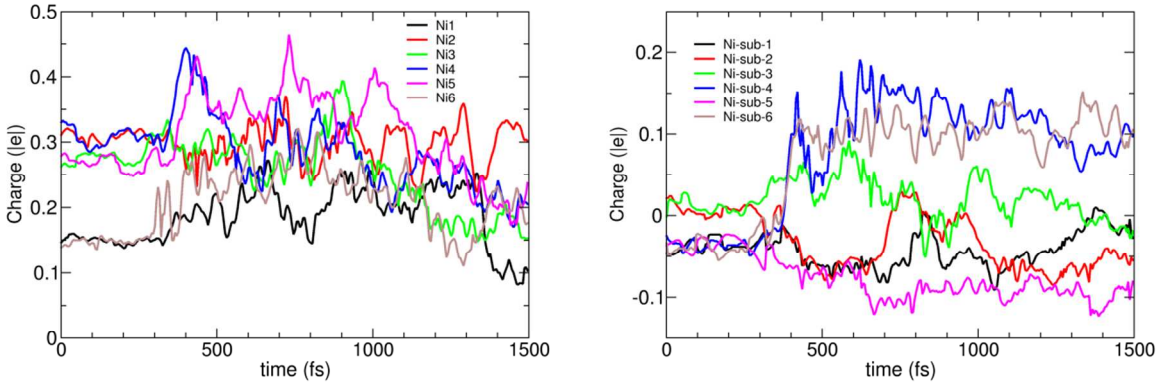

Figure S6. Atomic Bader charges of **surface (left) and subsurface (right) Ni** for a trajectory which corresponds to the **$CH_2 + CO_2^* \rightarrow H^* + CH^* + CO_2$** reaction.

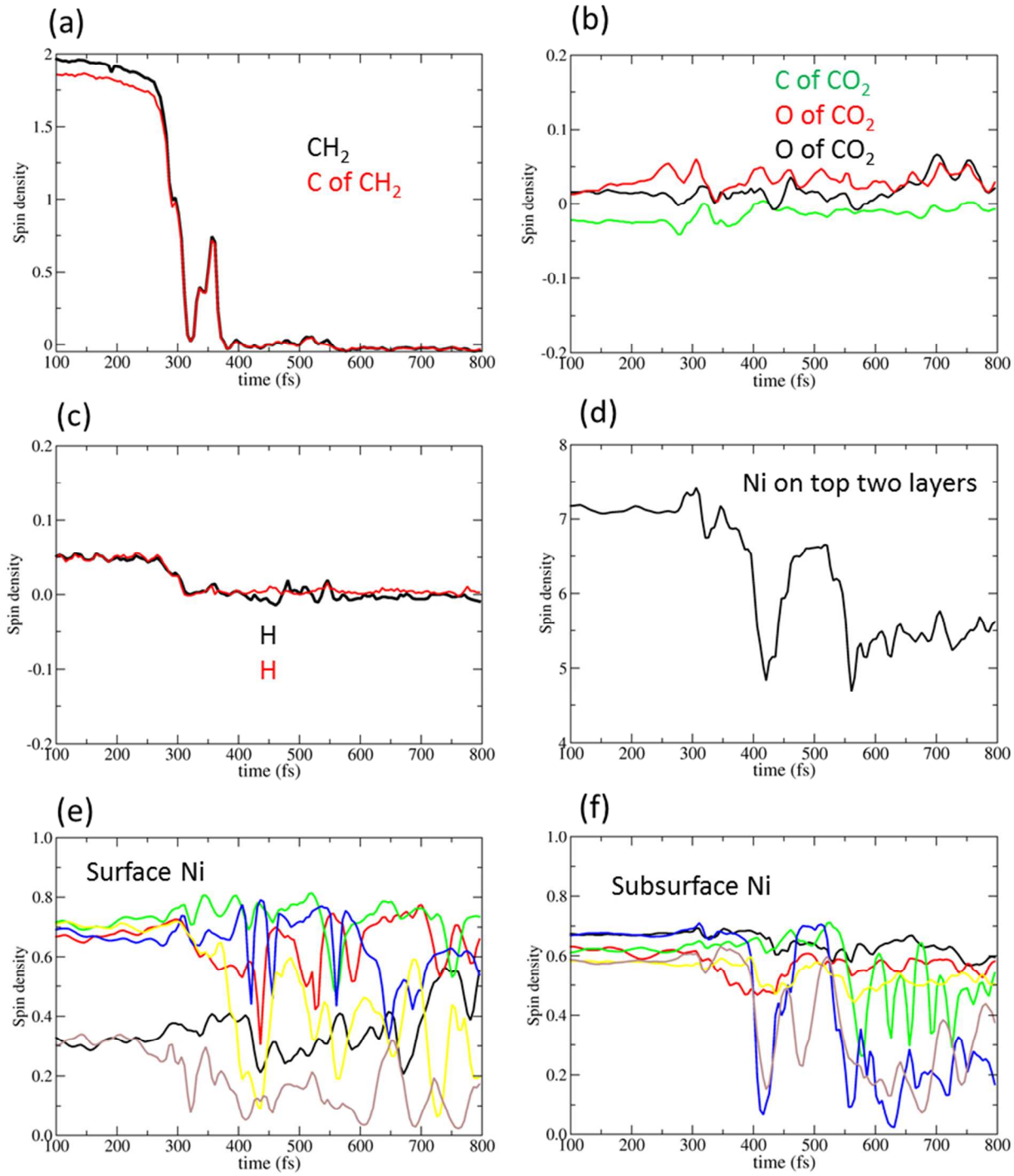

Figure S7. Evolution of spin densities for a trajectory which corresponds to the **$CH_2 + CO_2^* \rightarrow H^* + CH^* + CO_2$ (gas)** (Reaction 4 in Section 3.2 of the manuscript). Spin densities of (a) CH_2 and carbon in CH_2; (b) carbon of CO_2 and two oxygen atoms; (c) hydrogen atoms; (d) Ni on top two layers; (e) six surface Ni atoms; and (f) six subsurface Ni atoms.