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Supplementary Material

Preparation and Characterization of Silicon-Metal Fluoride Reactive Composites

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Combustion in Air

The adiabatic flame temperature and predicted mole fraction of the products of $50Si{\cdot}50CoF_2$ burning in air and calculated by NASA CEA code [1] are presented as a function of equivalence ratio in Figure S1. The calculations were performed for the constant pressure, 1 atm. The highest adiabatic flame temperature of 2750 K is predicted for the equivalence ratio range of 0.8–1.

In fuel-lean conditions ($\varphi << 1$) where lower adiabatic temperatures are expected, gaseous SiO was predicted to be the primary product with substantial gaseous F and Co species. The primary fluorinated product in the fuel-lean conditions is SiF_3. In fuel-rich conditions ($\varphi > 1$), representative of chemistry on the particle surface, considerable gasification of SiO_2 observed along with SiO. The primary fluorinated product is expected to be the thermodynamically stable SiF_4. Other fluorinated species such as HF and F are expected as well. Around the equivalence ratio of 0.8–1, the highest oxidation of silicon was observed with considerable gaseous and condensed phase SiO_2, along with products such as SiF_3 and SiF_4. The reduced cobalt could not be completely gasified across the range of equivalence ratios explored.

A similar calculation for $50Si{\cdot}50BiF_3$ was not run because thermodynamic data for bismuth species are lacking. A significant portion of the combustion products for $50Si{\cdot}50BiF_3$ is expected to be gaseous, facilitated by sufficiently high flame temperatures.

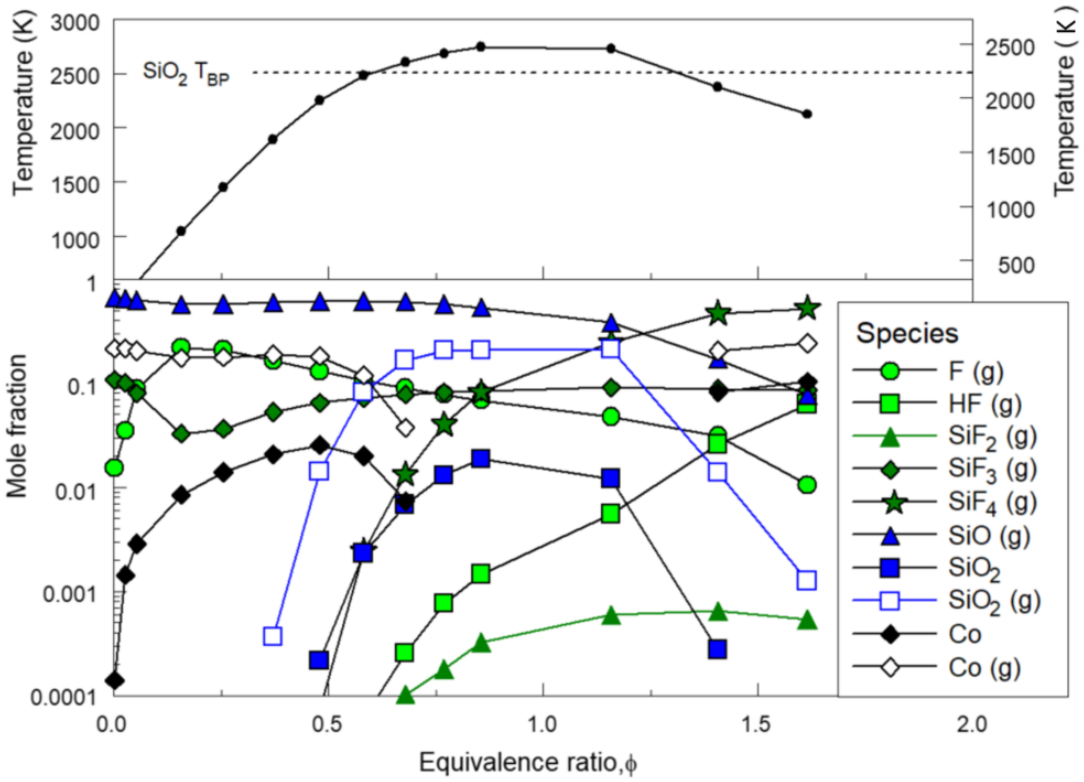

Figure S1. The calculated adiabatic flame temperature and the combustion products presented as mole fractions at a range of equivalence ratios for 50Si·50CoF_2.

References

1. McBride: B.J. and S. Gordon, *Computer Program for Calculation of Complex Chemical Equilibrium Compositions and Applications II. Users Manual and Program Description.* **1996**: NASA RP 1311, NASA Glenn Research Center, Cleveland, OH, USA.