

Chemical reaction networks relevant for cold molecules formation

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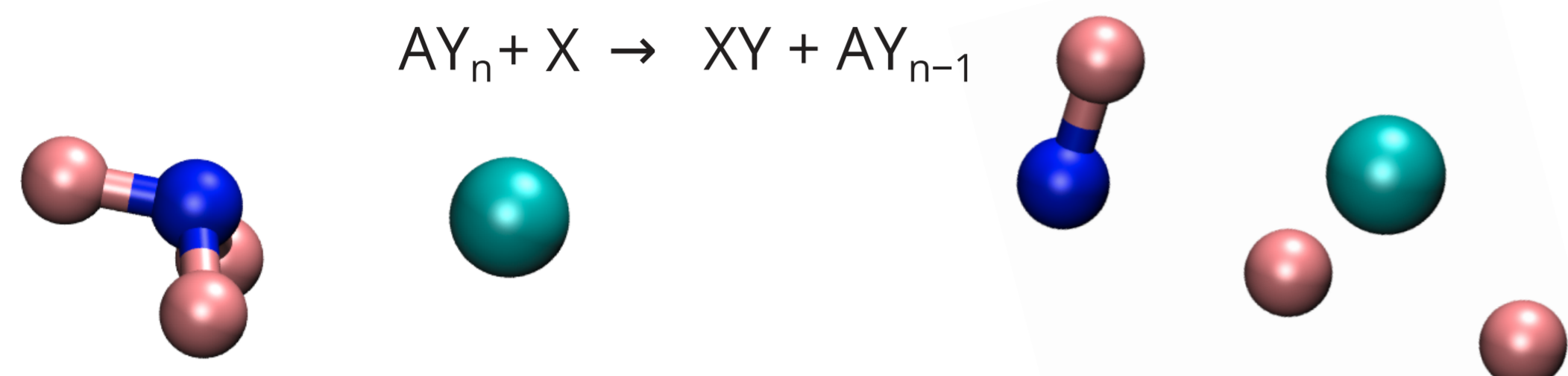
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INTRODUCTION

The impact of donor gas can be strong in collisions between an ablated metal X, in an atmosphere enriched with Y-donor gas



Target: The impact of initial collision energy of the ablated metal atoms on the reaction productivity

METHOD

Traditional transition state theory can not apply - The translational and vibrational states are absent.

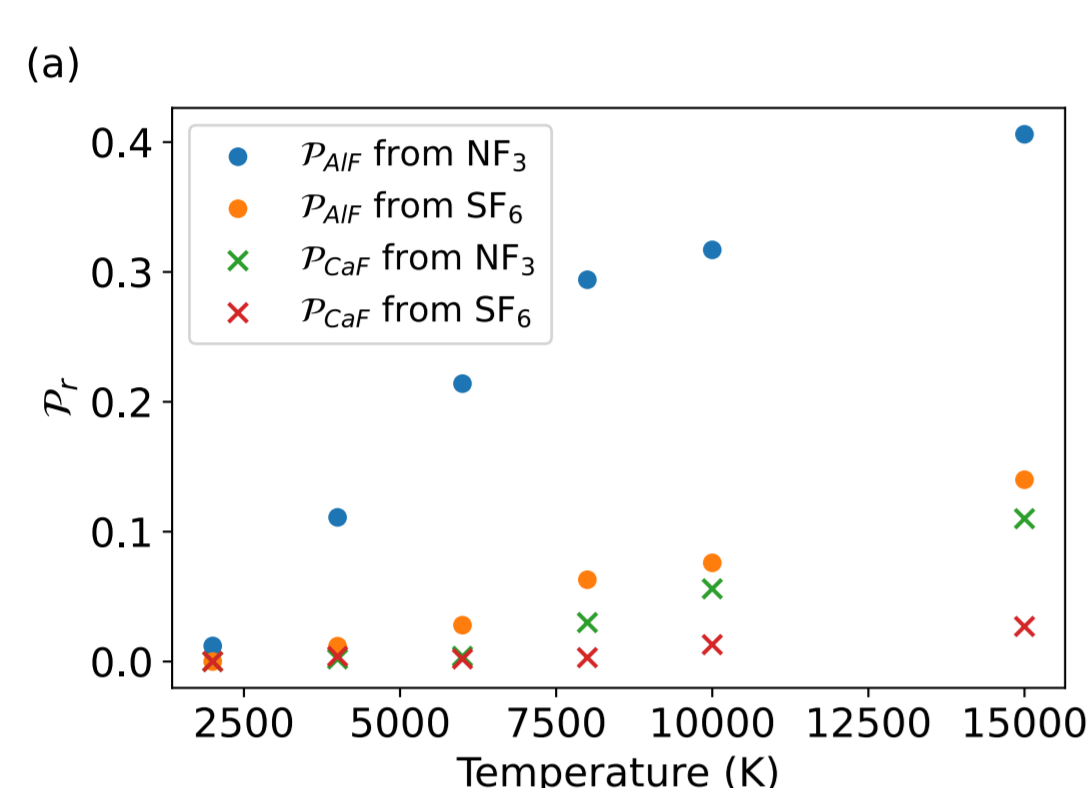
Impactical to construct the potential energy surface for an exact quantum dynamical treatment - The complexity increases drastically with the dimension.

→ **In this work:** *Ab initio* molecular dynamics simulations in the microcanonical ensemble at the B3LYP-D3/def2-TZVP level. The productivities of AIF and CaF are calculated from 1000 trajectories at each simulated temperature.

Tree-shaped Bayesian reaction networks have been constructed as directed acyclic graphs with the nodes being reactants, intermediates and products. The transition probabilities are obtained based on Bayesian inference.

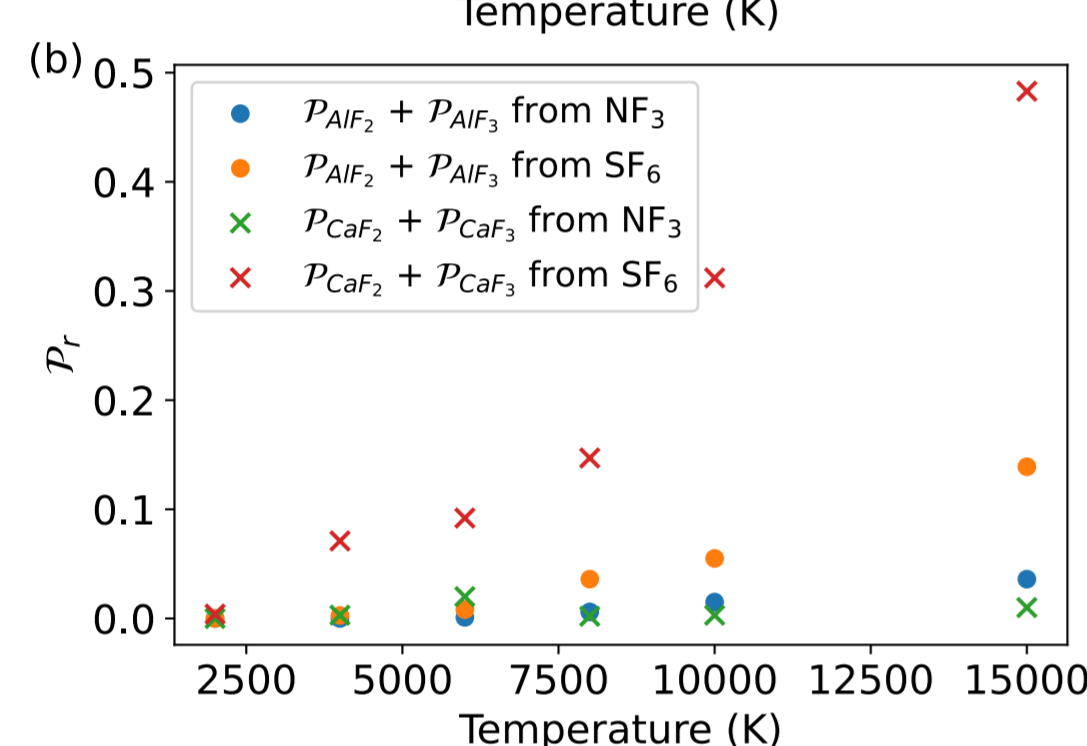
RESULT

Dependence of the productivity \mathcal{P} on donor gas and temperature



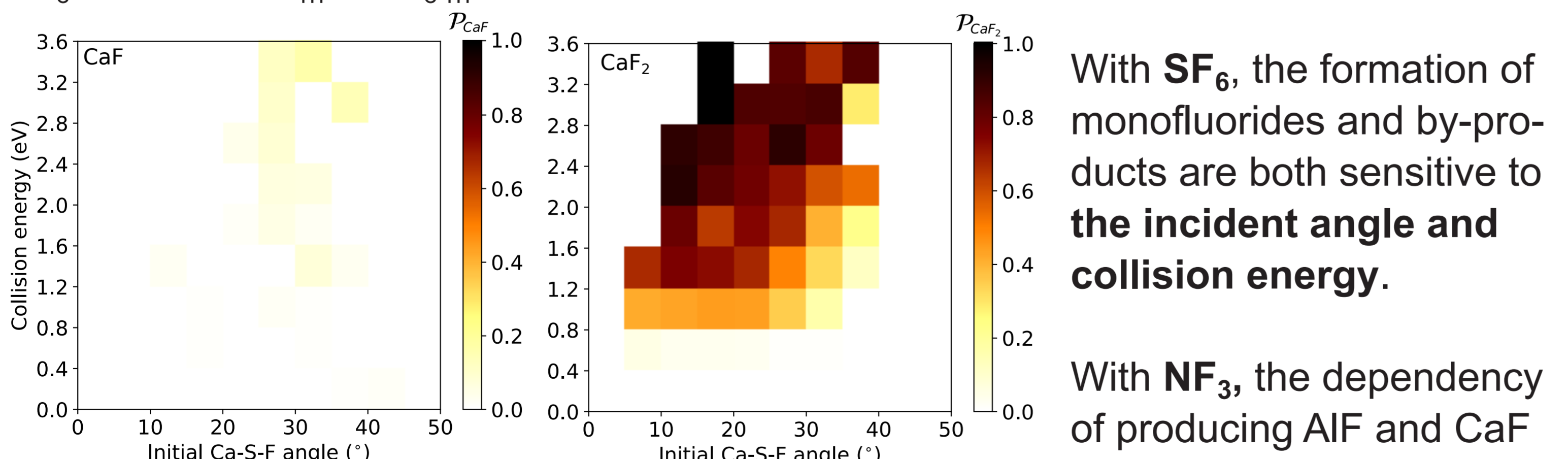
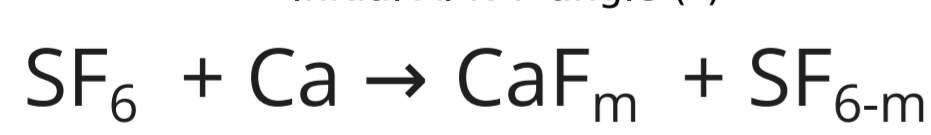
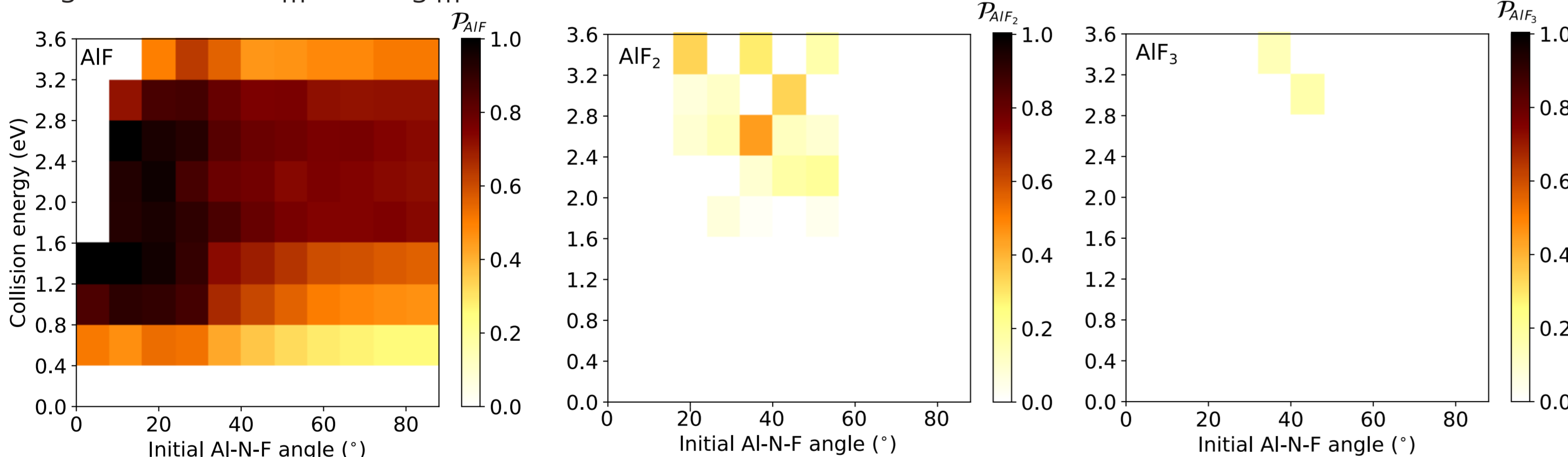
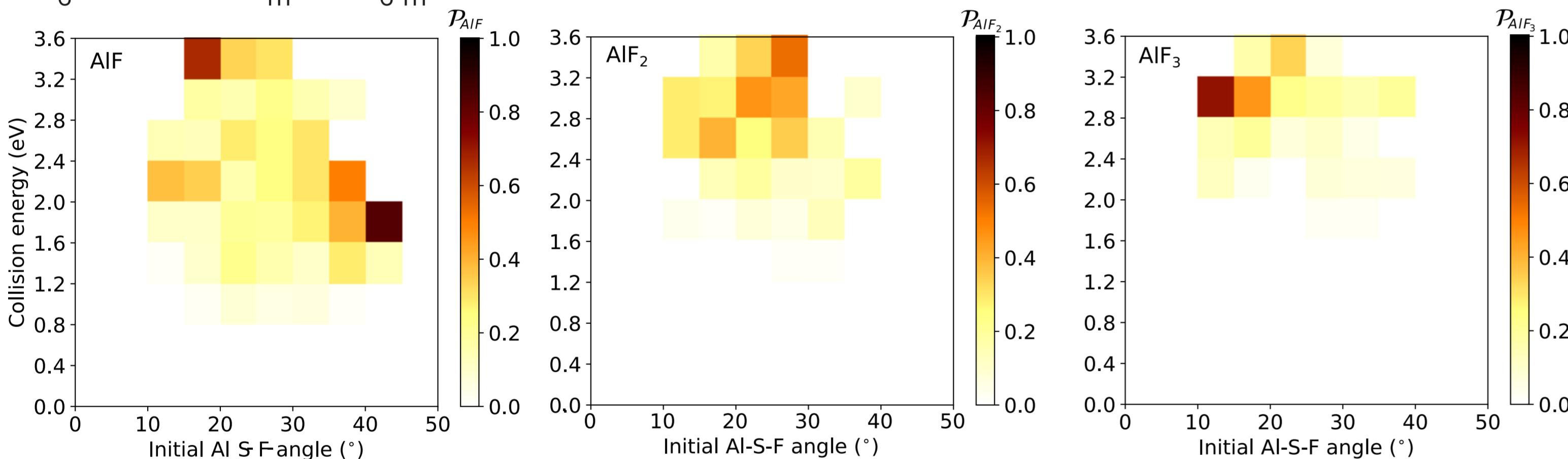
The choice of F-donor gas affects the reaction activity and selectivity.

The productivity and selectivity of **AIF** are an order of magnitude higher than **CaF**.



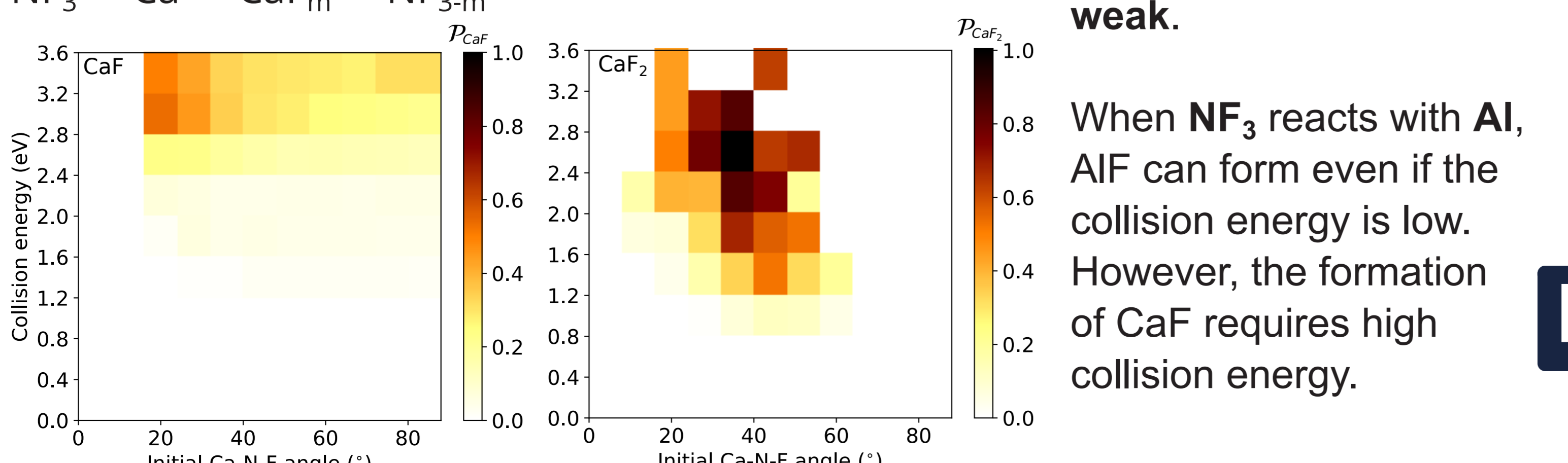
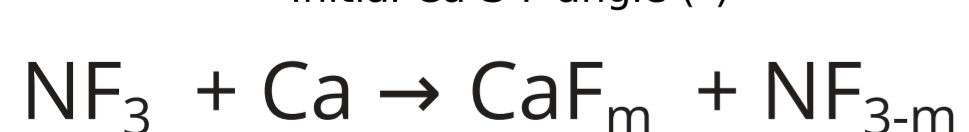
High temperature promotes the reactions forming monofluorides and by-products.

Dependence of the productivity \mathcal{P} on initial states



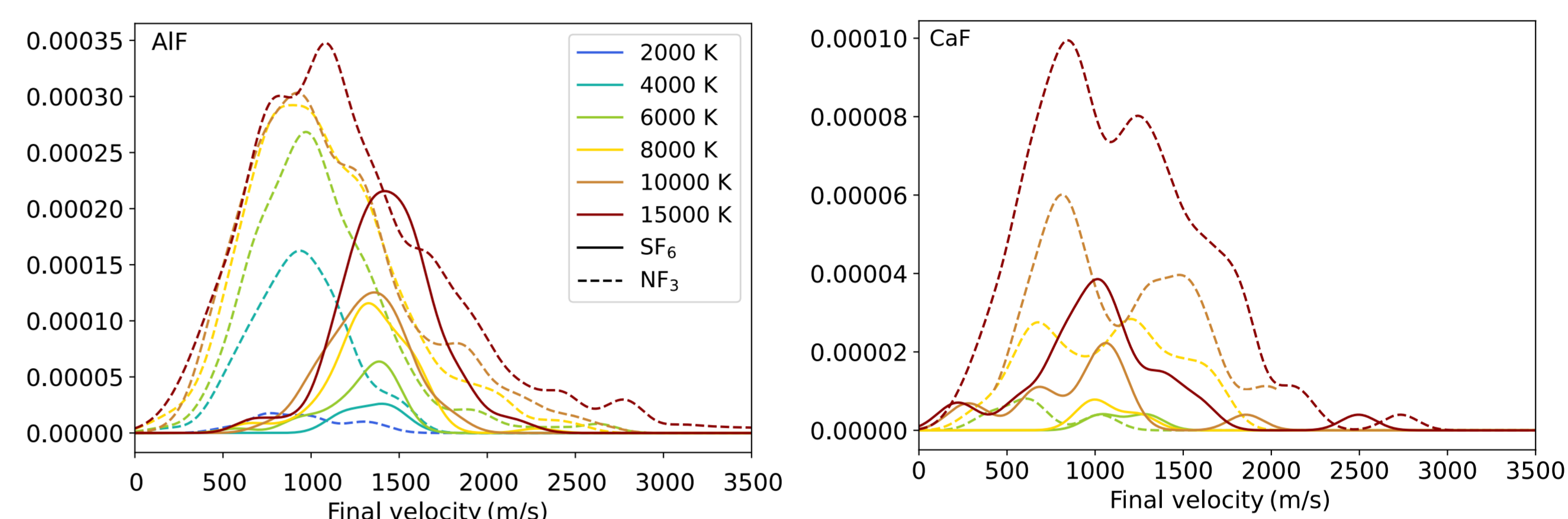
With **SF₆**, the formation of monofluorides and by-products are both sensitive to the incident angle and collision energy.

With **NF₃**, the dependency of producing AIF and CaF on the incident angle is weak.



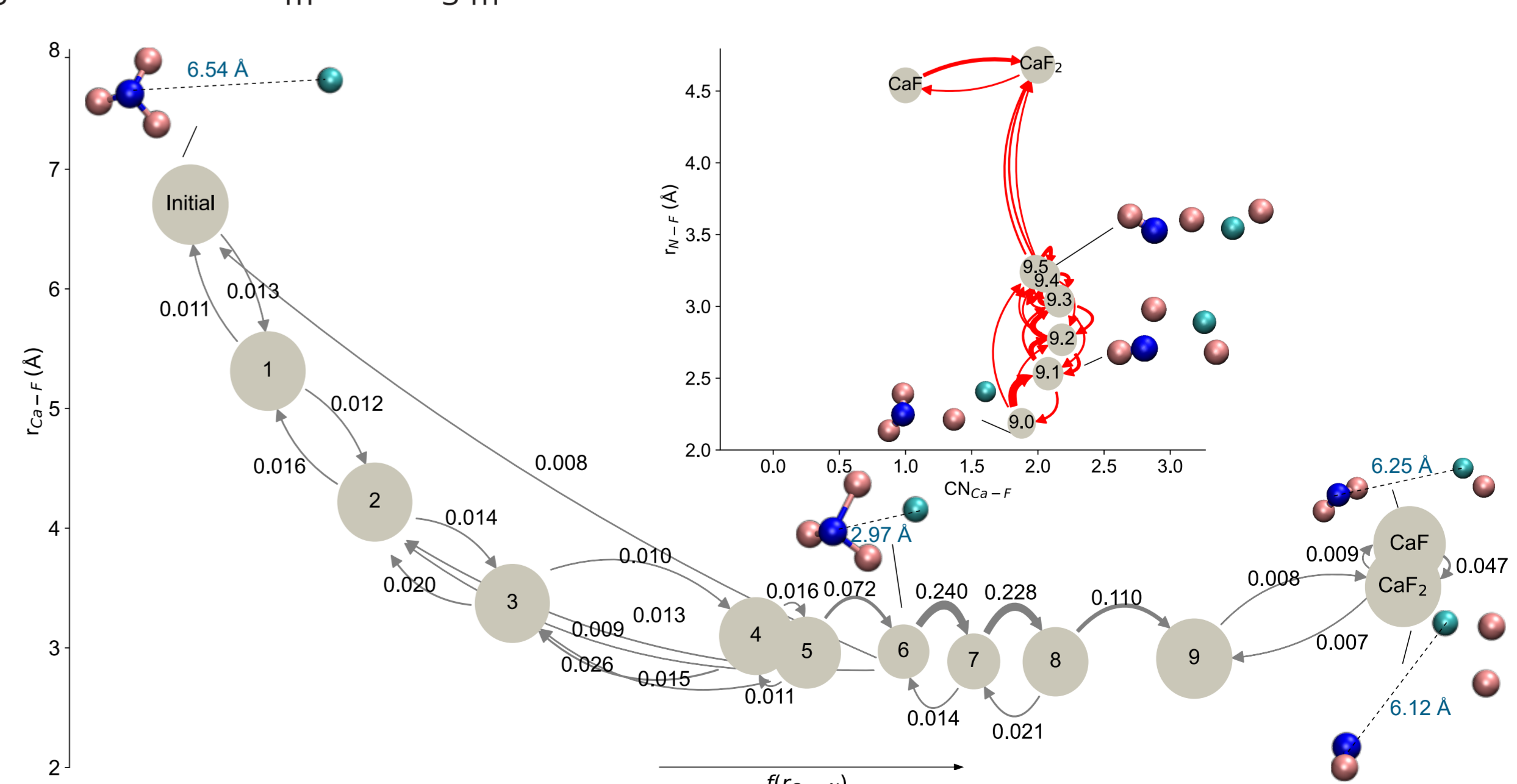
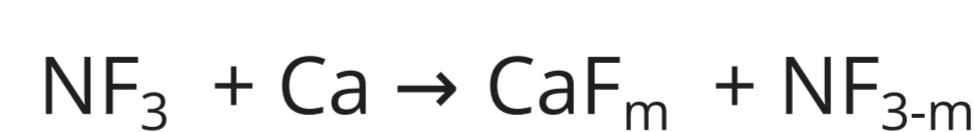
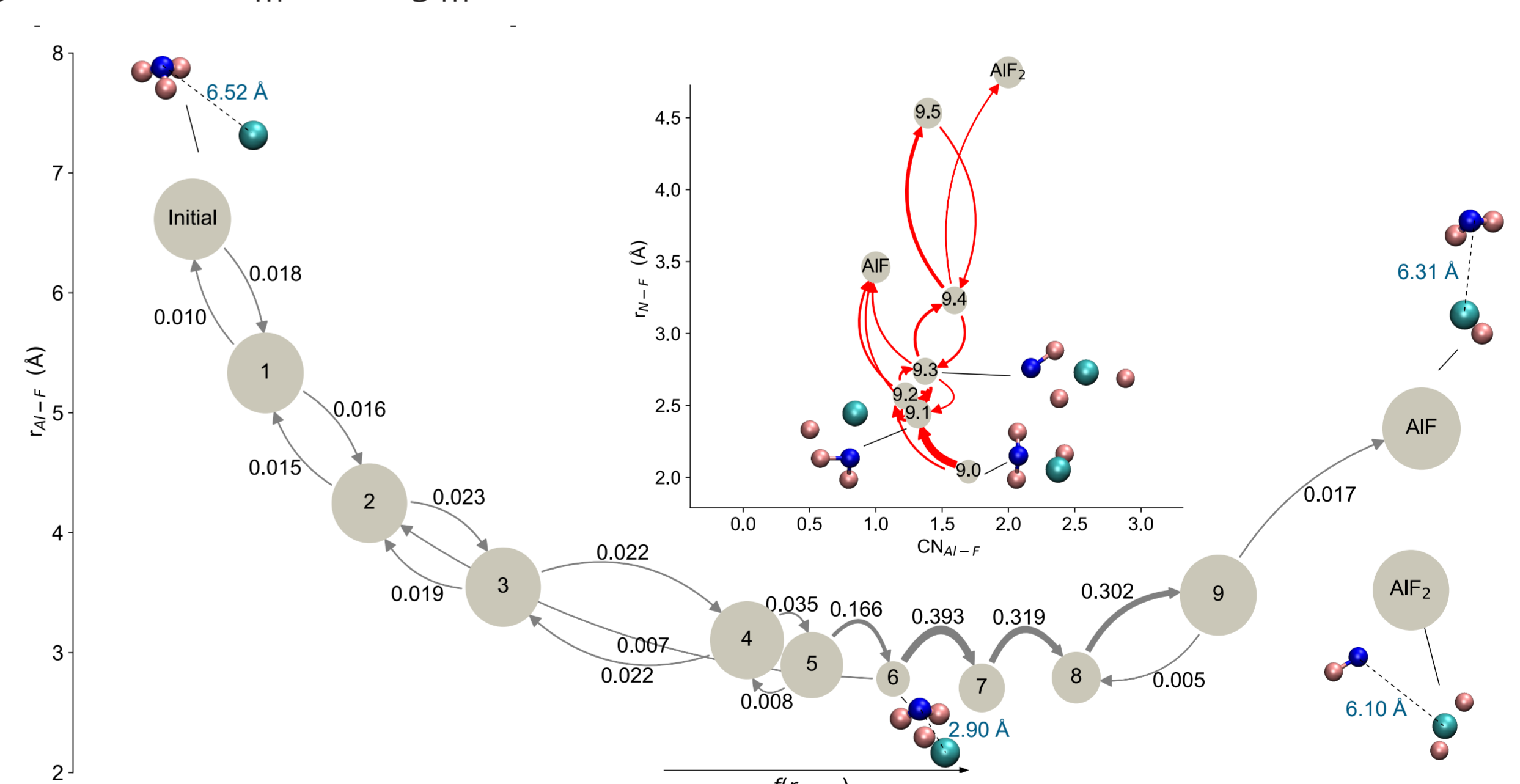
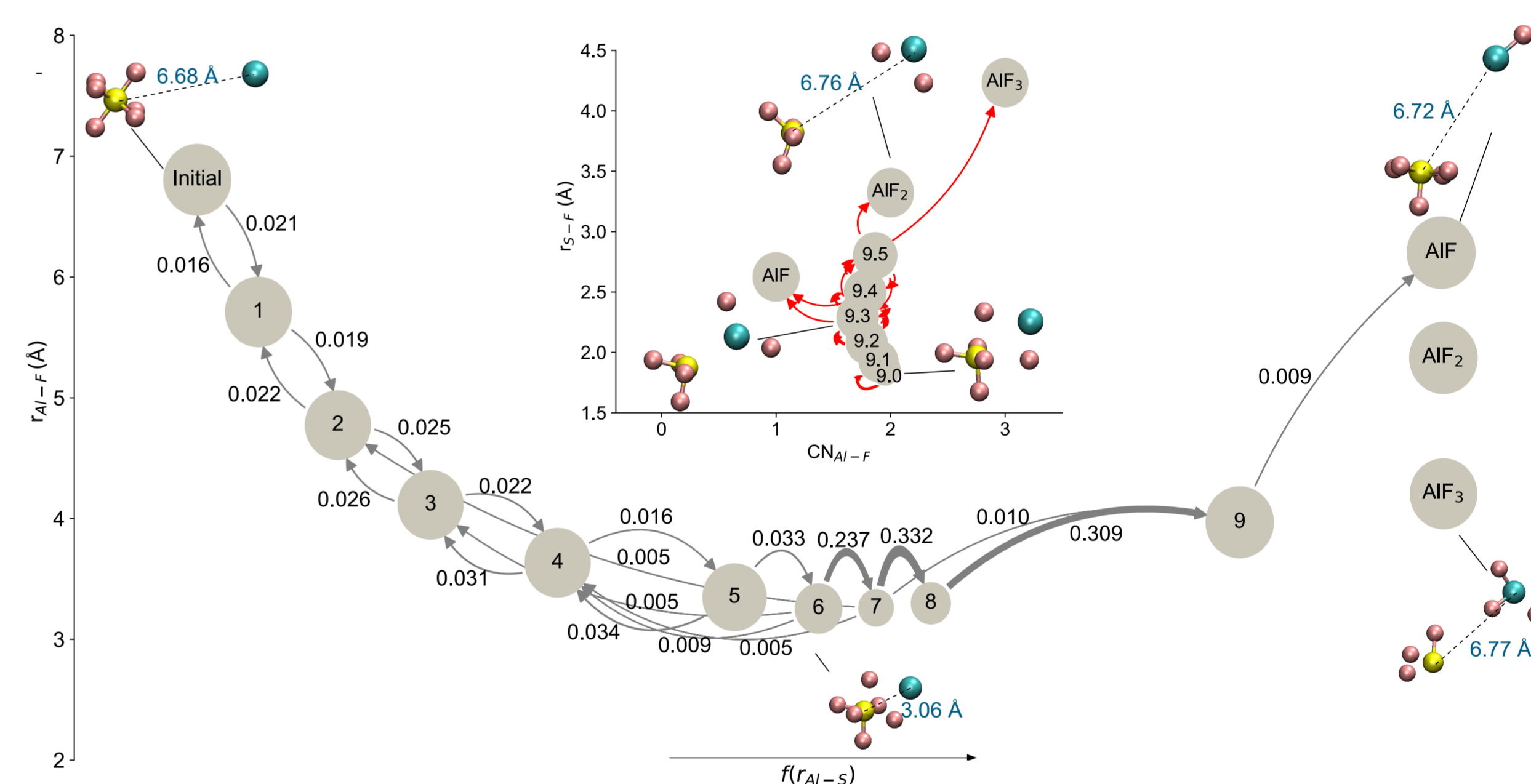
When **NF₃** reacts with **Al**, AIF can form even if the collision energy is low. However, the formation of CaF requires high collision energy.

Final velocity of the products



The final velocity of the products can be affected by the choice of F-donor gas. The distribution of final velocity can be influenced by temperature.

Tree-shaped Bayesian reaction networks



REFERENCE

[1] X. Liu, W. Wang, S. Wright, M. Doppelbauer, G. Meijer, S. Truppe, and J. Pérez Ríos, *J. Chem. Phys.* **2022**, 157, 074305.

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