Oxidation reaction dynamics of aluminum atoms at low and hyperthermal collisional energy

Fangfang Li#, Yujie Ma#, Dong Yan, Ang Xu, Jiaxing Liu, Fengyan Wang*

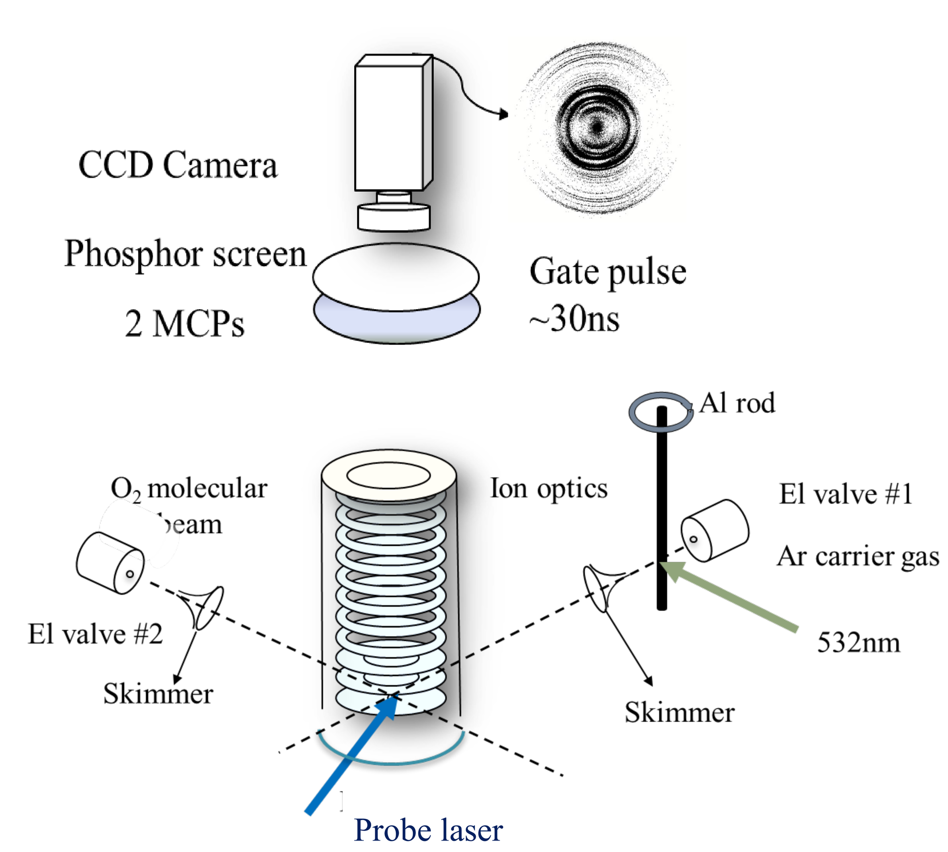
Department of Chemistry and Shanghai Key Laboratory of Molecular Catalysis and Innovative Materials, Collaborative Innovation Center of Chemistry for Energy Materials (iChEM), Fudan University, Shanghai 200433, China

Abstract

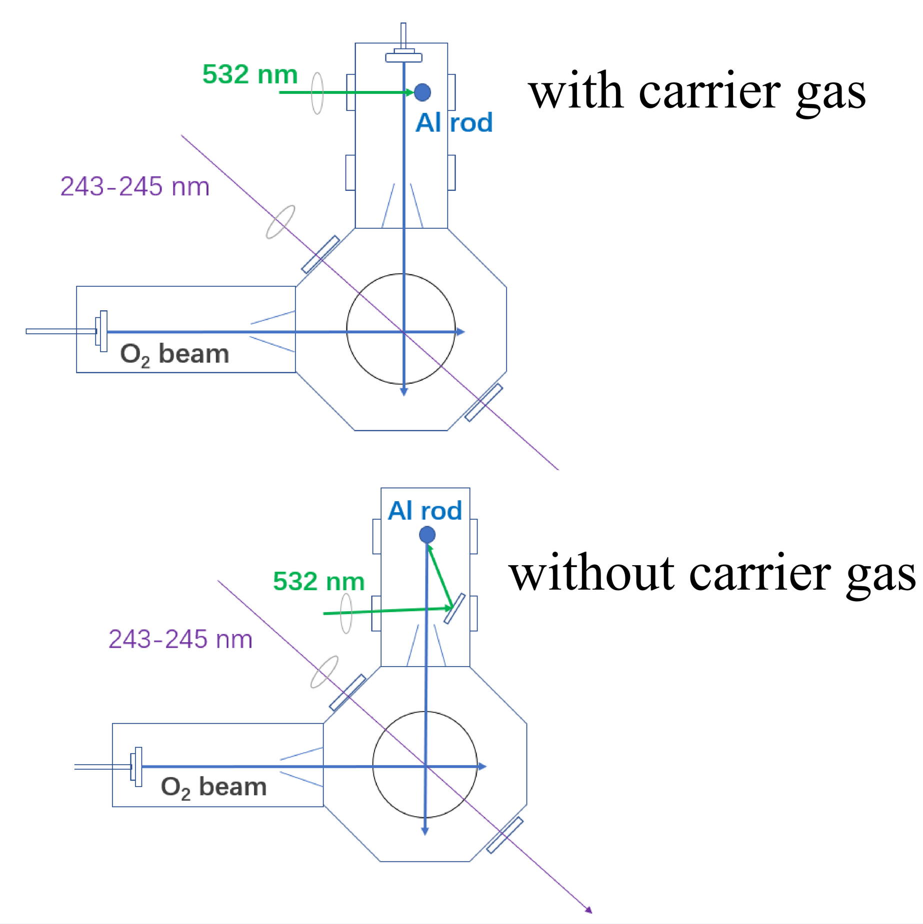
Using the time-sliced ion velocity imaging and crossed molecular beam apparatus, where the metal atomic beam can be generated with or without using buffer carrier gas, we studied the reaction dynamics of $Al(^2P)+O_2(X^3\Sigma^+)\rightarrow AlO(X^2\Sigma^+)+O(^3P_J)$ in the collision energy range of around 1.5 -20 kcal/mol. At a low collision energy of 1.45 kcal/mol, the Al atomic beam is generated by 532 nm laser ablation of the Al metal rod, carried out by Ar carrier gas to form a supersonic metal atomic beam, and then collides with O_2 molecular beam. When no carrier gas is used and the laser ablation metal beam is directly sprayed into the reaction chamber, the ultra-fast aluminum atoms at 3000 m/s can be obtained. Under this condition, the oxidation reaction of aluminum atoms at the high collisional energy of 20.0 kcal/mol was studied. At low collisional energy, the product angular distributions characterized by the forward-backward peaks and the preference in the forward direction indicate the existence of AlO_2 complex with the lifetime comparable to its rotational period; while at high collisional energy, the observation with the strong backward-scattering angular distribution of AlO products indicates that the direct oxidation reaction occurs at low impact parameters.

Experimental method

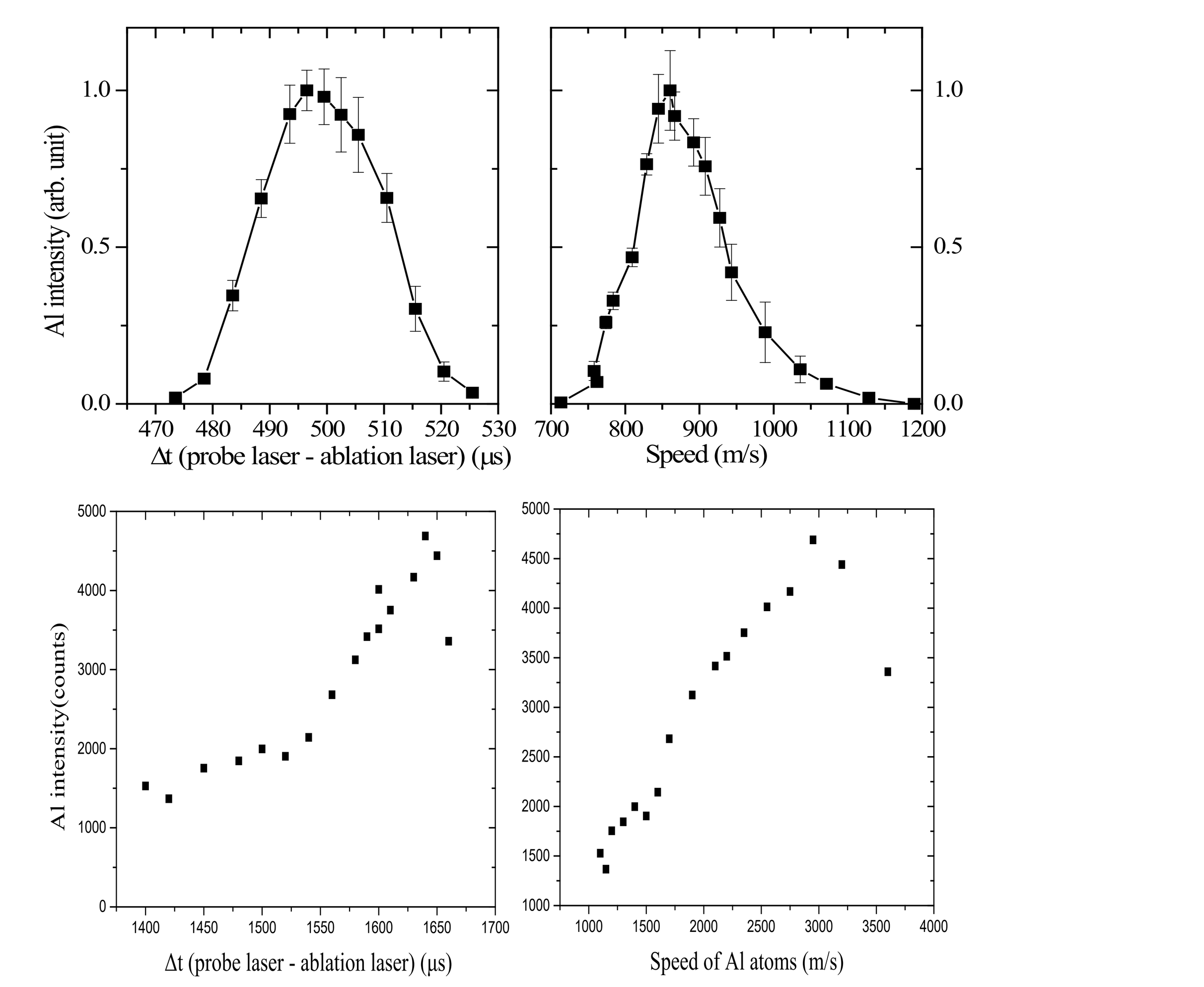
(a) Crossed-beam and time-sliced ion velocity imaging setup



(b) Metal atomic beam with/without carrier gas



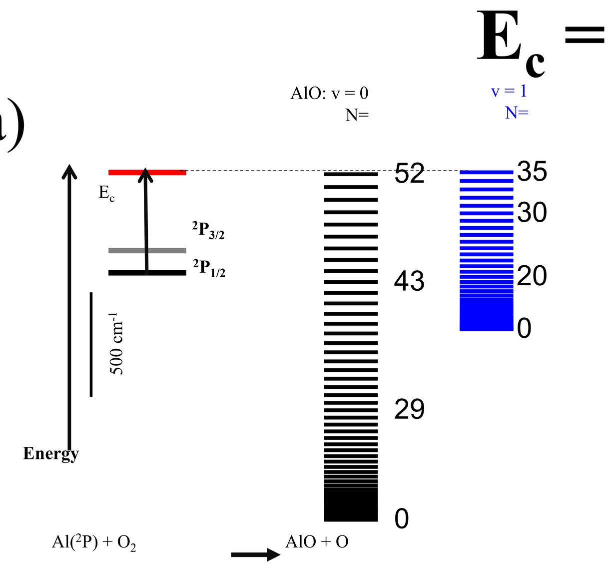
(c) Speed distribution of Al atomic beam



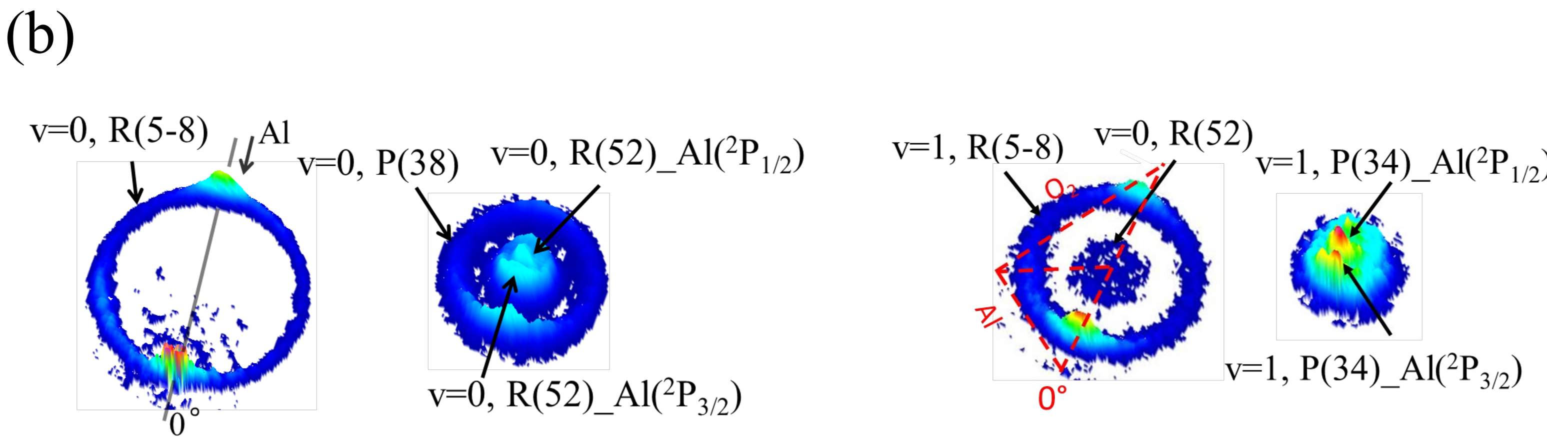
Studies of $Al(^2P) + O_2(X^3\Sigma^+) \rightarrow AlO(X^2\Sigma^+) + O(^3P_J)$ reaction

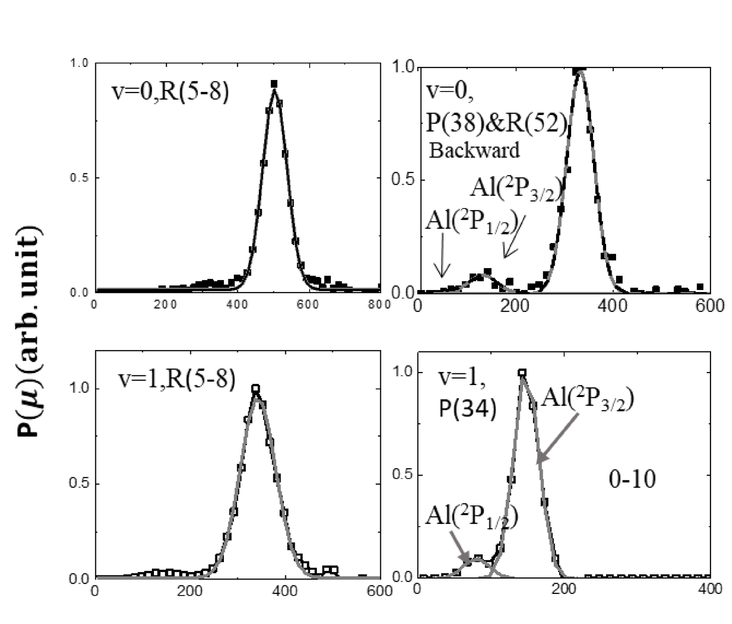
E_c = 1.45 kcal/mol

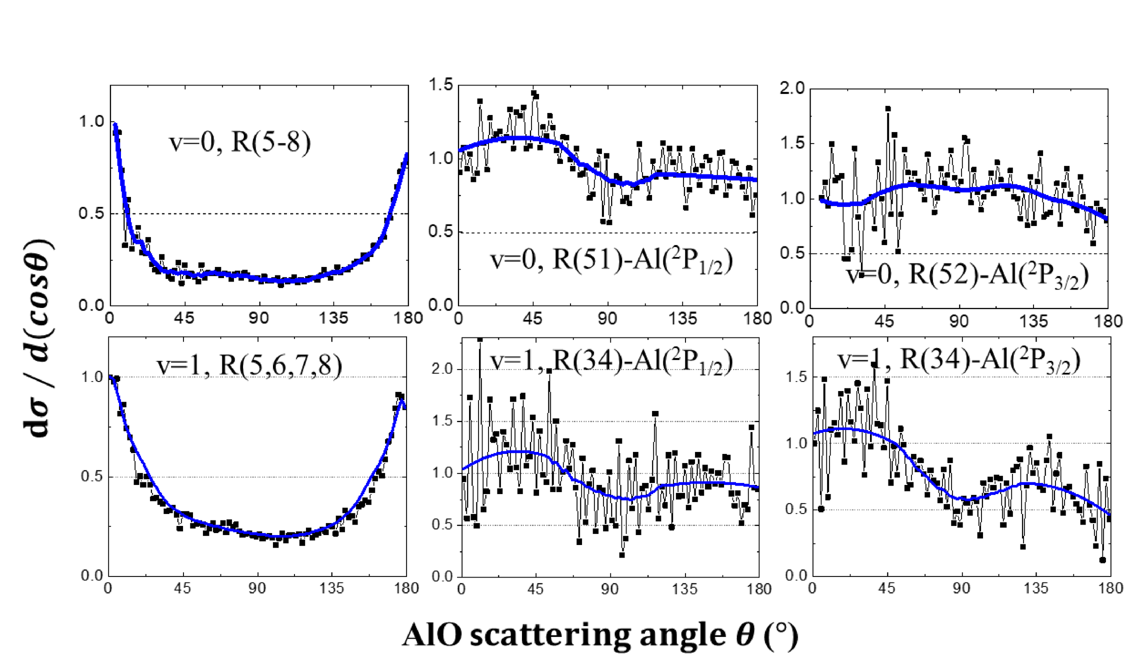
(a)



(b)

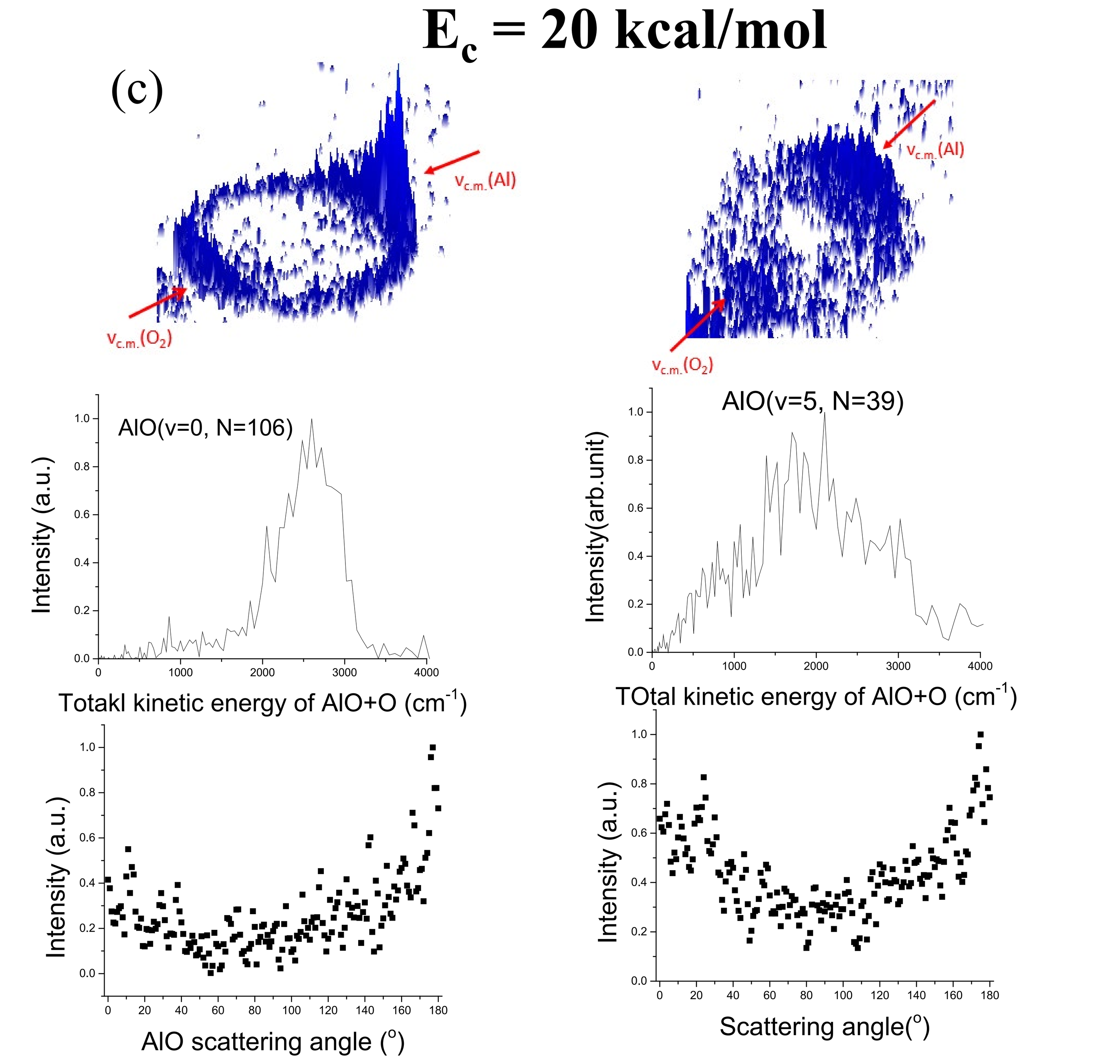






E_c = 20 kcal/mol

(c)



(a) The energetics data for the reaction of $Al(^2P_J) + O_2(X\ ^3\Sigma^-_g) \rightarrow AlO(X\ ^2\Sigma^+) + O(^3P_J)$ at the collisional energy Ec = 1.5kcal/mol. (b) The raw images of the $AlO(X\ ^2\Sigma^+$, v = 0 and1) products at various rotational levels N(N=5-8, N=52 and N=34) are obtained with corresponding velocity and angular distributions of AlO products. The product angular distributions characterized by the forward-backward peaks and the preference in the forward direction indicate the existence of AlO_2 complex with the lifetime comparable to its rotational period.

(c) At high collisional energy of ~20 kcal/mol the slice images of AlO products are obtained with corresponding velocity and angular distributions of AlO products. . The observation with the strong backward-scattering angular distribution of AlO products indicates that the direct oxidation reaction occurs at low impact parameters.

References

[1] A. Xu et al., *Chin. J. Chem. Phys.* **34**, 61 (2021).
[3] F.F. Li et al., *Chemical Science.* **9**, 488 (2018).
[2]Y.Ma et a., *J. Phys. Chem. A.* **123**,3672(2019).
[4] H.Pan et al., *J. Phys. Chem. A.* **124**,6573(2020).

Acknowledgments

This work was supported by the National Natural Science Foundation of China (No. 22073019 and 21673047), the Shanghai Key Laboratory Foundation of Molecular Catalysis and Innovative Materials, and the Program for Professor of Special Appointment (Eastern Scholar) at Shanghai Institutions of Higher Learning.