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First-Principles Exploration of the Competing Mechanisms for the Sign Preference in Ion-induced Nucleation LIUBIN XU, WEI CHEN, PING CUI, ZHENYU ZHANG, University of Science and Technology of China —
Ion-induced nucleation plays an important part in aerosol formation, under both atmospheric and experimental conditions. However, the dominant mechanism underlying the so-called sign preference, a phenomenon that ions of the same magnitude of charge but opposite signs exhibit notably different enhancement of nucleation, remains an enigma. Recent experiments revealed a negative charge affinity of 1-propanol molecules condensing on tungsten oxide seeds, while prevailing first-principles calculations indicated a positive preference. In this study, we investigate the adsorption of organic molecules on charged transition metal oxide via density functional theory (DFT) calculations by including new physical factors that were absent in previous theoretical studies. First, we demonstrate the significant role of van der Waals interactions in such systems. Furthermore, we show that the change of charge state effectively varies the spin moment of the seeds, which can be utilized to selectively influence the strengths of the intermolecular bindings. These new factors may prove to be instrumental in gaining an eventual complete understanding of the long-standing sign preference puzzle in ion-induced nucleation.

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