

STICKING COEFFICIENTS OF SOME KEY GASEOUS SPECIES ON ATMOSPHERIC AEROSOLS DERIVED FROM QUANTUM MECHANICAL CALCULATIONS

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Adsorption of atmospheric gases such as NO, NO₂, HNO₃,... on various aerosols surfaces has been mainly pointed out from chamber experiments. Some of these experiments allowed to deduce their uptake coefficients which may be dependent on the experimental conditions (time exposure, particle size and concentration, temperature ...). Another approach results from the a-priori calculation of the interaction energy and dynamics of molecules from the gas phase at surfaces. In this context we present calculated values of the sticking coefficients of some key atmospheric compounds i.e., NO, NO₂, ozone,... on soot aerosols. These values are obtained from quantum mechanical calculations based on specific implementations of Density Functional Theory. The theoretical approach is general and applicable to the sticking of molecular species on sea salt particles and mineral aerosols.