Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

for

Reaction Probability and Kinetics of H_2O Splitting on the Penta-$NiAs_2$ Monolayer from an Ab Initio Molecular Dynamics Investigation

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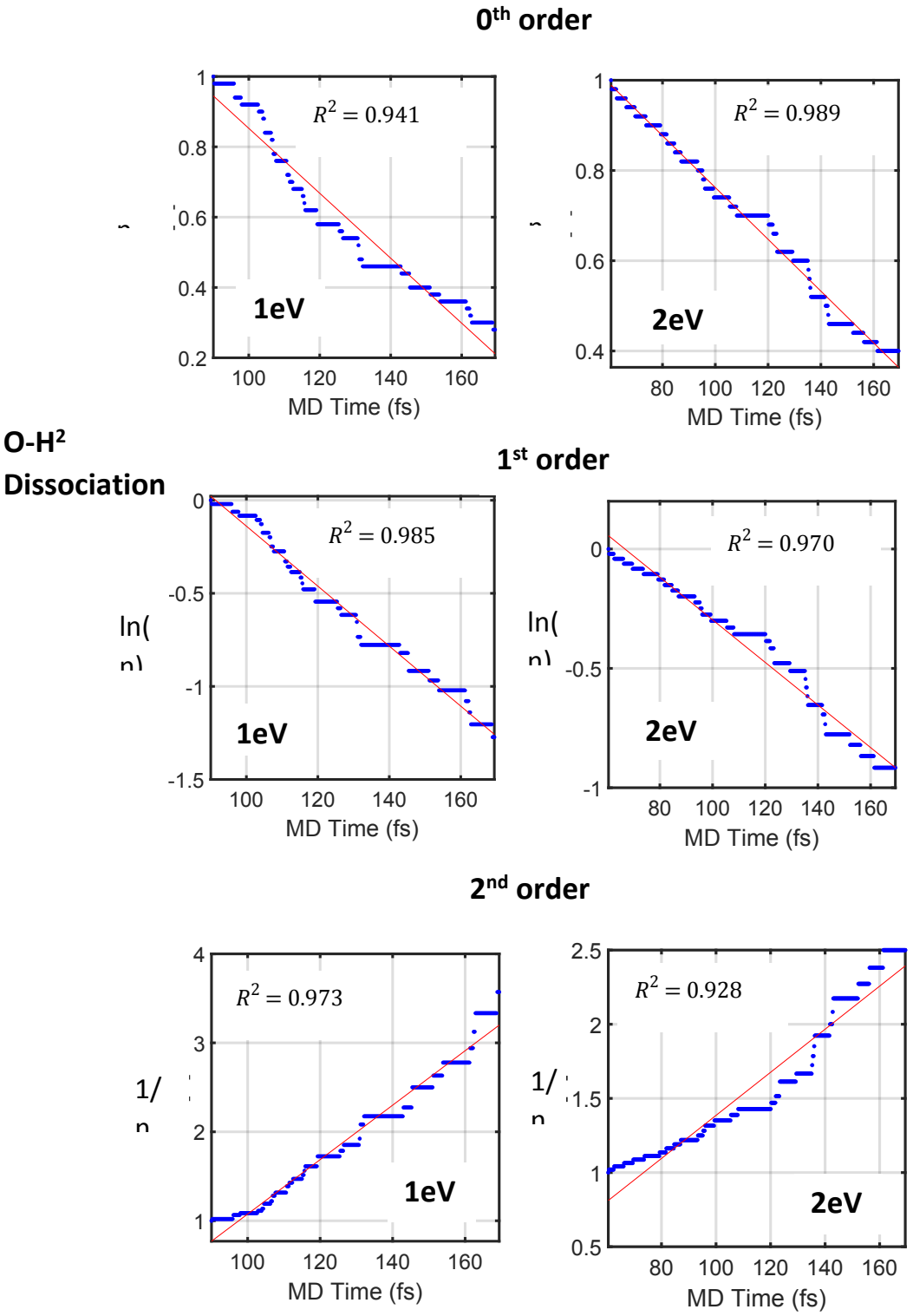

Figure S1: Fitting plots for rate constant of the first O-H dissociation with respect to initial kinetic energy of 1 eV (left panel) and 2 eV (right panel) for zeroth, first, and second order types, respectively. In each plot, n is the concentration ratio of remaining H_2O samples with respect to MD time. The red lines represent the fitting line and blue dots are actually data.

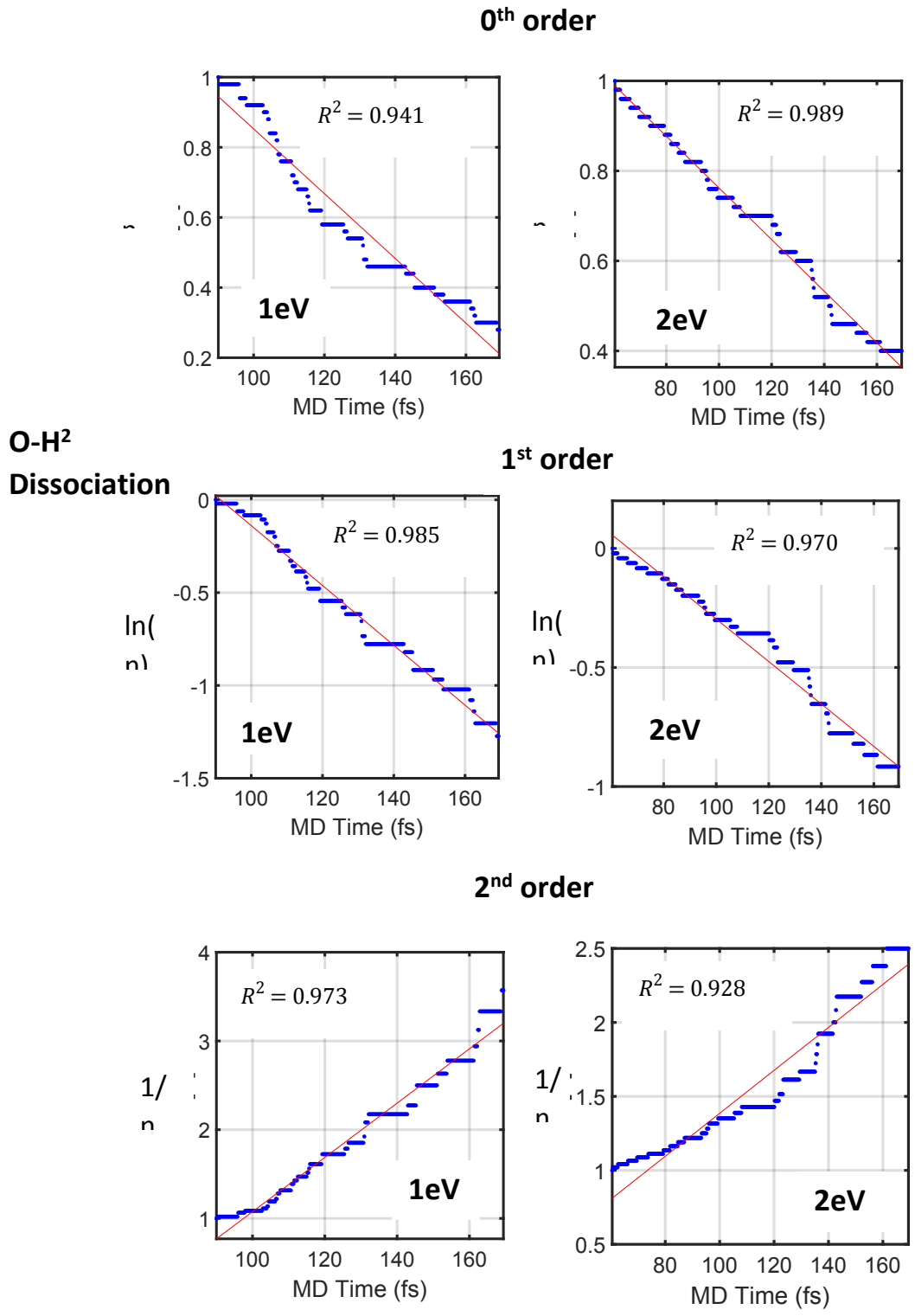

Figure S2: Fitting plots for rate constant of the second O-H dissociation with respect to initial kinetic energy of 1 eV (left panel) and 2 eV (right panel) for zeroth, first, and second order types, respectively. In each plot, n is the concentration ratio of remaining H_2O samples with respect to MD time. The red lines represent the fitting line and blue dots are actually data.

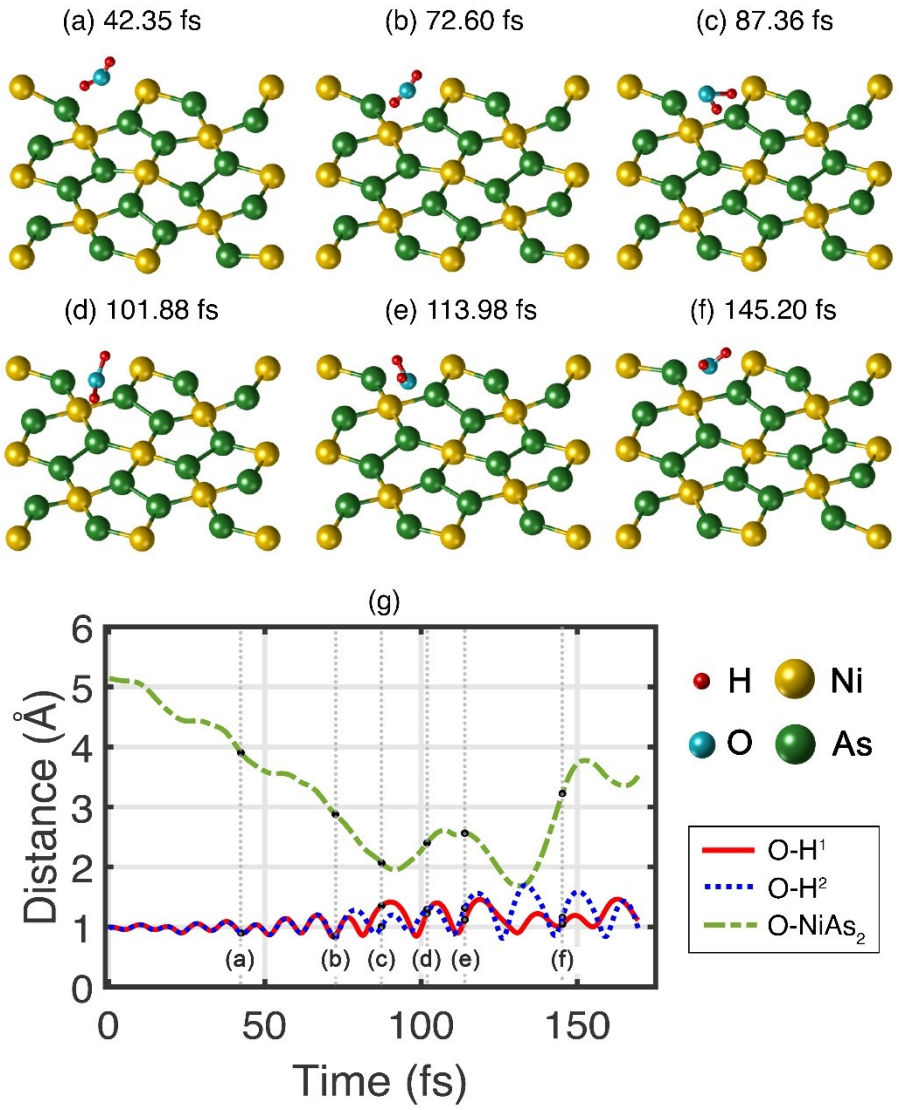

Fig. S3 (a)-(f) Snapshots of the H_2O molecule on the $NiAs_2$ surface for a non-reacting case, (g) two O-H distances (red solid and blue dotted lines) and projected distance between O and the $NiAs_2$ surface (green dashed line) with respect to time. The black dots and vertical lines indicate selected configurations shown in (a)-(f).