of-freedom when a metal cluster is deposited on an Ar surface[35, 36]. One can define a dipole energy which scales as the square of the dipole amplitudes. Figure 11 shows a typical result for the time evolution of the energy contained in the oscillating dipoles in the case of reflection of Na_6 deposited on MgO. There is a small initial value which corresponds well to the finite initial distance of the Na cluster to the substrate. There is a large contribution at the time of closest impact. This part is dominated by (instantaneous) static polarization which would also be contained in a Born-Oppenheimer MD. The dipole energy falls back to lower values when the cluster departs from the substrate (see figure 6). But there remains some offset which corresponds to the energy finally transferred to the dipole degrees of freedom. It amounts to about 2% of the impact energy, which is small compared to the other energetic observables, see figure 14 and corresponding discussion in section III D 3. In contrast to the case of Ar substrate, energy transfer to MgO dipoles has actually only a small effect for the overall ionic dynamics. But more subtle properties as optical response and trajectories of free charges (to be discussed in a subsequent publication) will be sensitive to such details.

2. *Energy transfers "at" impact*

Notwithstanding asymptotic thermalization, the fast energy transfer to the substrate in the early stages is an interesting observable characterizing the collision process. Figure 12 shows the kinetic energy of the substrate

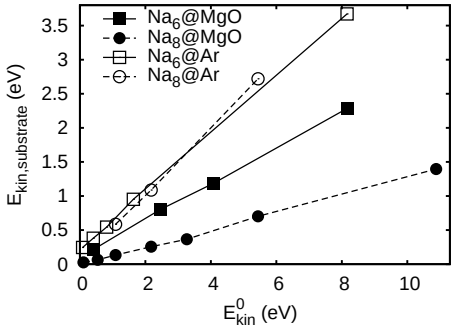

FIG. 12: Heating of the MgO or Ar substrate after impact of Na_6 and Na_8. The energy transfer to Ar is independent of the cluster structure, whereas the energy transfer to MgO is not. Na_6 transfers about twice as much energy as the compact Na_8.

soon after the collision, i.e. averaged over the first 2 ps after impact, as a function of the initial kinetic energy of the cluster $E^0_{\rm kin}$. Apparently the energy absorbed by the substrate is proportional to $E^0_{\rm kin}$. But the slope depends very much on cluster and surface types. The soft Ar substrate absorbs much more energy than MgO, typically a bit more than 50% of the initial kinetic energy. The softness and the rather small surface corrugation of Ar make the process insensitive to the actual cluster which is approaching. That is different for MgO. There is always less energy absorption by the substrate and there is a strong dependence on the cluster configuration. Na_6 transfers more than twice as much energy as Na_8. The strong surface corrugation of MgO induces that sensitivity to cluster geometry. Remind that Na_6 does not match very well to the MgO surface while Na_8 does (see section II F).

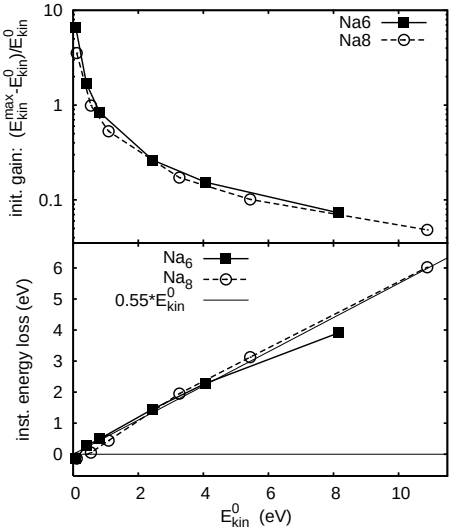

FIG. 13: Upper panel : The gain in kinetic energy of the cluster when approaching the MgO surface; lower panel : Instantaneous energy loss, defined as the difference between maximum kinetic energy before the impact and next maximum after impact.

More information about what is happening directly around impact time can be obtained by reading off observables at shorter time scales (shorter than the 2 ps used above). Figure 13 shows two such observables as a function of initial kinetic energy. The upper panel shows the energy gain in the approaching phase due to the acceleration by the polarization potential. It is defined as the difference of the first maximum of the cluster kinetic energy and the initial energy. Na_6 acquires slighlty more energy than Na_8 because it has a non-vanishing dipole moment which, in turn, enhances the polarization attraction. There is a large gain in the low energy range (the regime of soft deposit), while the trend becomes very flat for fast collisions. This is probably due to a move from adiabatic to non-adiabatic relaxation processes in the surface. For very low impact velocities, the surface ions have time to follow the forces from the cluster, whereas for very high velocities the surfaces ions do not have enough time to respond before the cluster collides. The lower panel of figure 13 shows an attempt to quantify an "instantaneous energy loss". To that end, we take difference between the maximum kinetic energy before the impact and the next maximum after the impact. Obviously the instantaneous energy transfer is practically the