

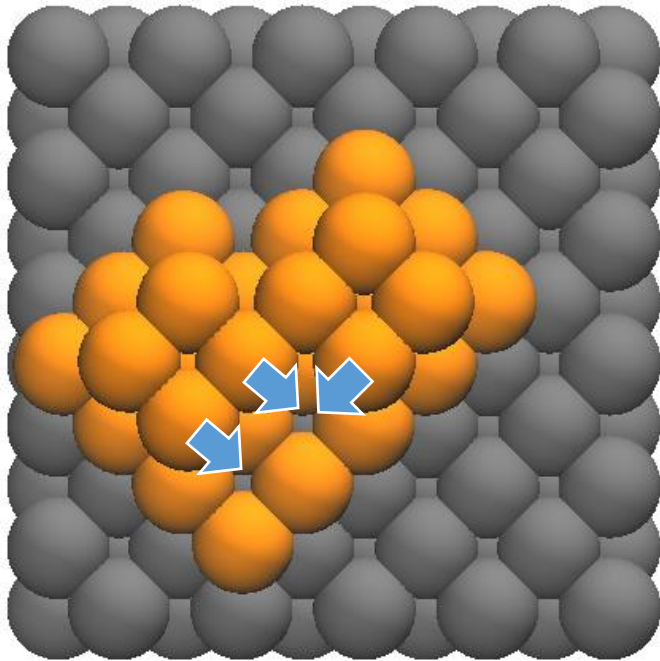
SUPPLEMENTARY MATERIAL FOR “**Uncertainty Quantification of Kinetic Monte Carlo Models constructed on-the-fly using Molecular Dynamics**”

Abhijit Chatterjee\*

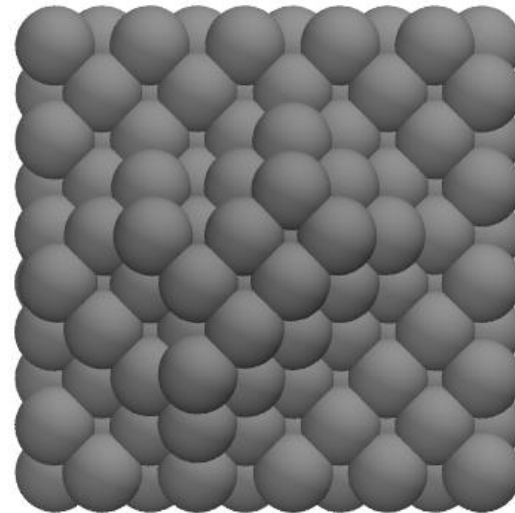
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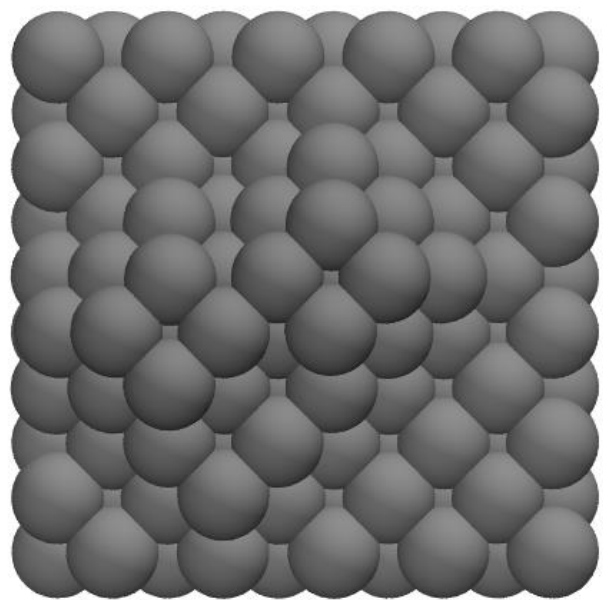
EXAMPLES OF MOVES ENCOUNTERED IN THE DYNAMICAL EVOLUTION OF THE Ag NANOCUSTER (see main text)



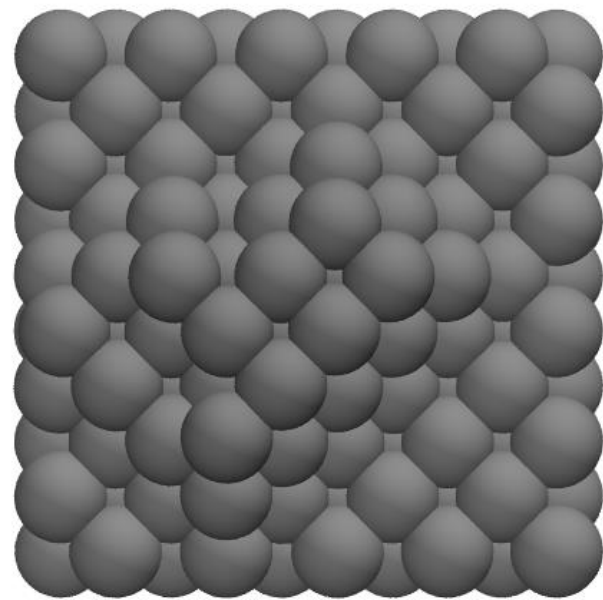
Ag/Ag(001)  
Initial state



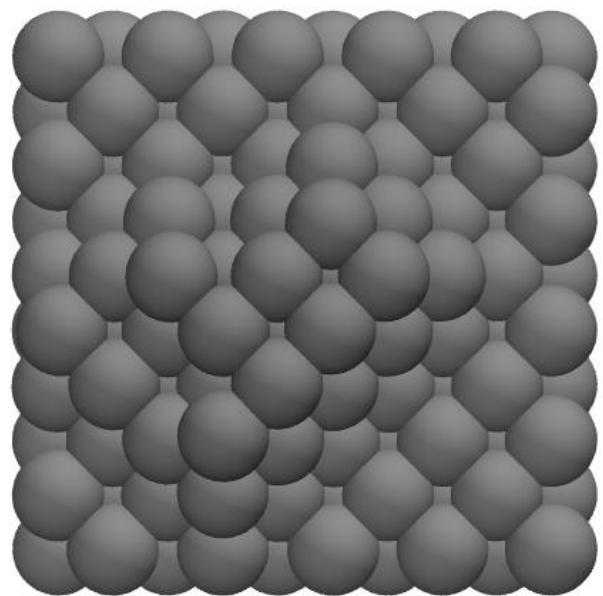
Hop process  
in a different state



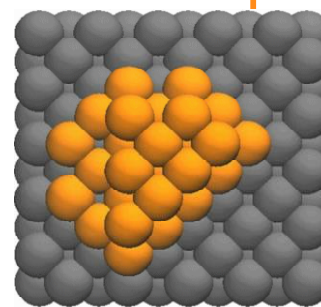
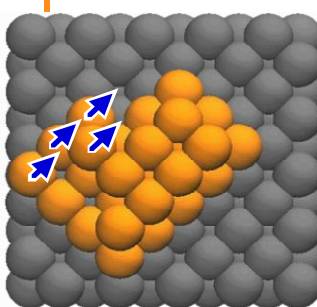
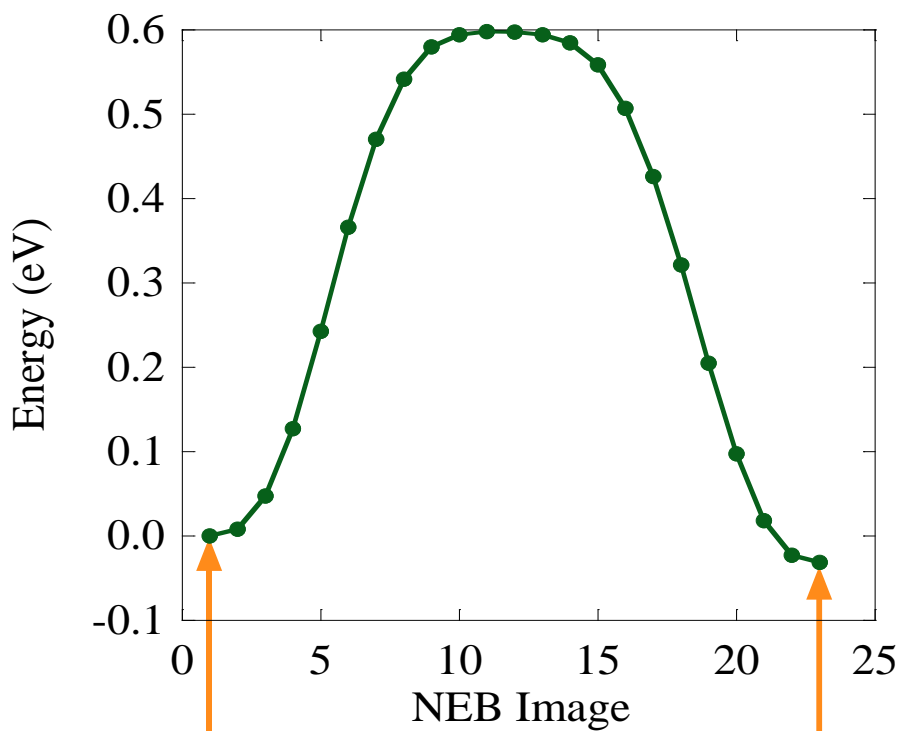
Two atom exchange

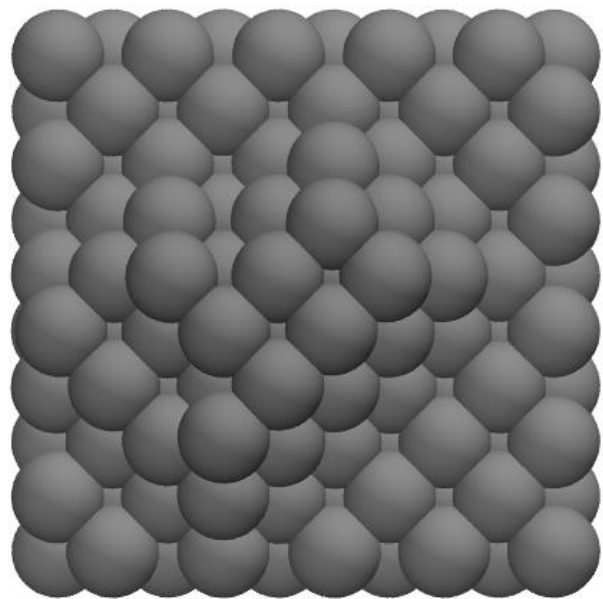


Two atom hop

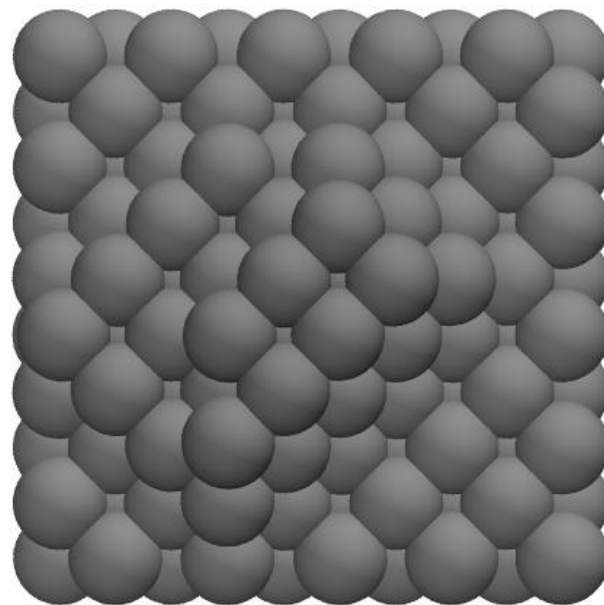


4-atom slide mechanism



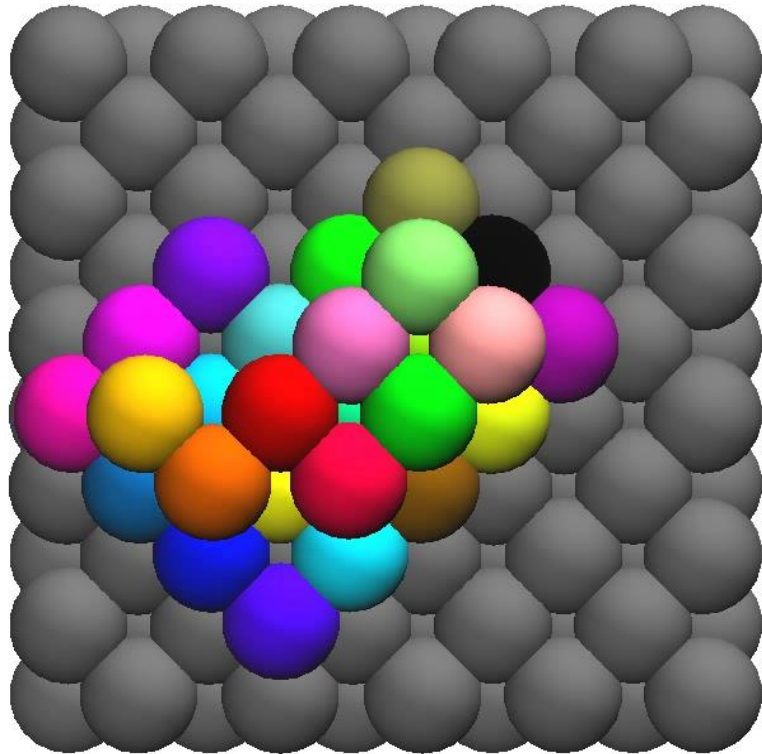


5-atom process  
Off-lattice



8-atom slide mechanism  
Off-lattice

A movie showing the state-to-state dynamics obtained with the KMC model for the Ag nanocluster on Ag(001) surface is provided. The grey-coloured atoms denote the substrate atoms. Nanoparticle atoms are shown in different colours to aid our understanding of the processes that are selected in the KMC dynamics. Several concerted moves are selected in the KMC dynamics.



	<p>Single-atom hop moves where the atoms run along an edge, such as the move shown, have low barriers and are selected frequently. These moves play a minor role in the overall restructuring of the 3D nanoparticle to a 2D cluster. We call these moves the edge-</p>
<p>running moves.</p>	
	<p>However, two-atom hop moves can also be fast. They are selected multiple times as seen in the first 12 seconds of the movie.</p>
	<p>Here the atoms are packed in a compact structure and the hop moves have a large barrier. A single atom climbs up a step while overcoming the Schwoebel barrier. The move does not play an important role in the overall dynamics.</p>
	<p>Similarly, the yellow atom climbs down even though an edge-running atom is present. This move is observed after 35 s after a long sequence of edge-running moves.</p>
	<p>At 42s into the movie we find two unusual moves one after the other. The dark blue atom climbs up a step. The move is followed by a three-atom move, such that the orange and the dark blue atom descend to the lower layer. Another atom is also displaced in the process.</p>