# Supplementary Online Information for: Beam induced heating in electron microscopy modeled with machine learning interatomic potentials

Cuauhtemoc Nuñez Valencia[1], William Bang Lomholdt[2], Matthew Helmi Leth Larsen[1], Thomas W. Hansen[2], and Jakob Schiøtz[1]

[1]Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark.

[1]National Centre for Nano Fabrication and Characterization, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark.

## 1 Learning curve

Figure SOI-1 shows how the RMSE error of the forces depend on the training set size. The curve is obtained by randomly picking subsets of the full training set, and shows that beyond 2000 configurations in the training set no further improvement is seen.

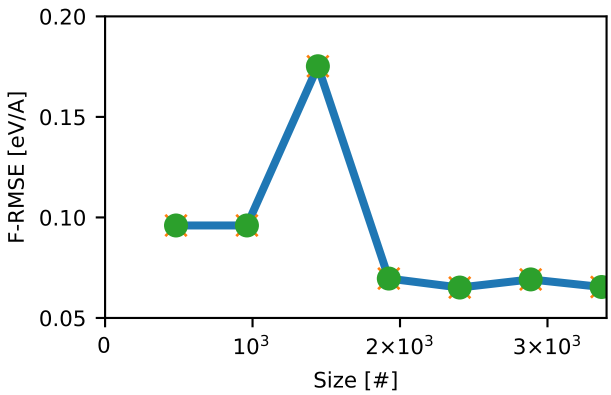


Figure SOI-1: Learing curve: The RMSE force error in the validation set as a function of the training set size (the validation size was the same for all the models).

## 2 Surface area ratio

The ratio between the contact area for thermal conductivity ($A$) and the transverse area presented to the beam may vary by more than an order of magnitude, see Fig. SOI-2.

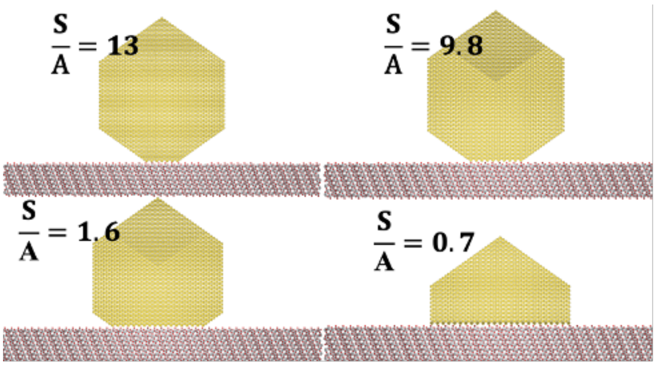


Figure SOI-2: Depending on the wetting angles, the $S/A$ ratios can vary by an order of magnitude or more.

## 3 Importance of unrealistically large forces when training

In principle, the potential should be able to extrapolate the configuration with relatively large forces on the atoms without any problem. In the figure SOI-3 we can see how diverse is our training set in the magnitude of the force, most of the dataset lies with relative small forces (between 0–2 eV/A), however the error versus magnitude of the force is a relative flat curve (see lower panel figure SOI-3) which means that the model is also able to predict large forces; the errors in large forces (between 3–5eV/A) are around twice the average of the error in the small forces(between 0–1eV/A).

Given that we are interested in modelling systems that on average have relatively small forces (between 0–5 eV/A), the majority of our training set lie in this range. However, we trained a model where the training set only contains forces below 5 eV/A; we can see that the results are significantly worse than for a model trained with the same training set size but not excluding the small fraction of configurations with large forces (Figure SOI-3, lower panels). We speculate that this is because it is important for the neural network to see atomic configurations that would not be well described by a harmonic approximation near a local energy minimum.

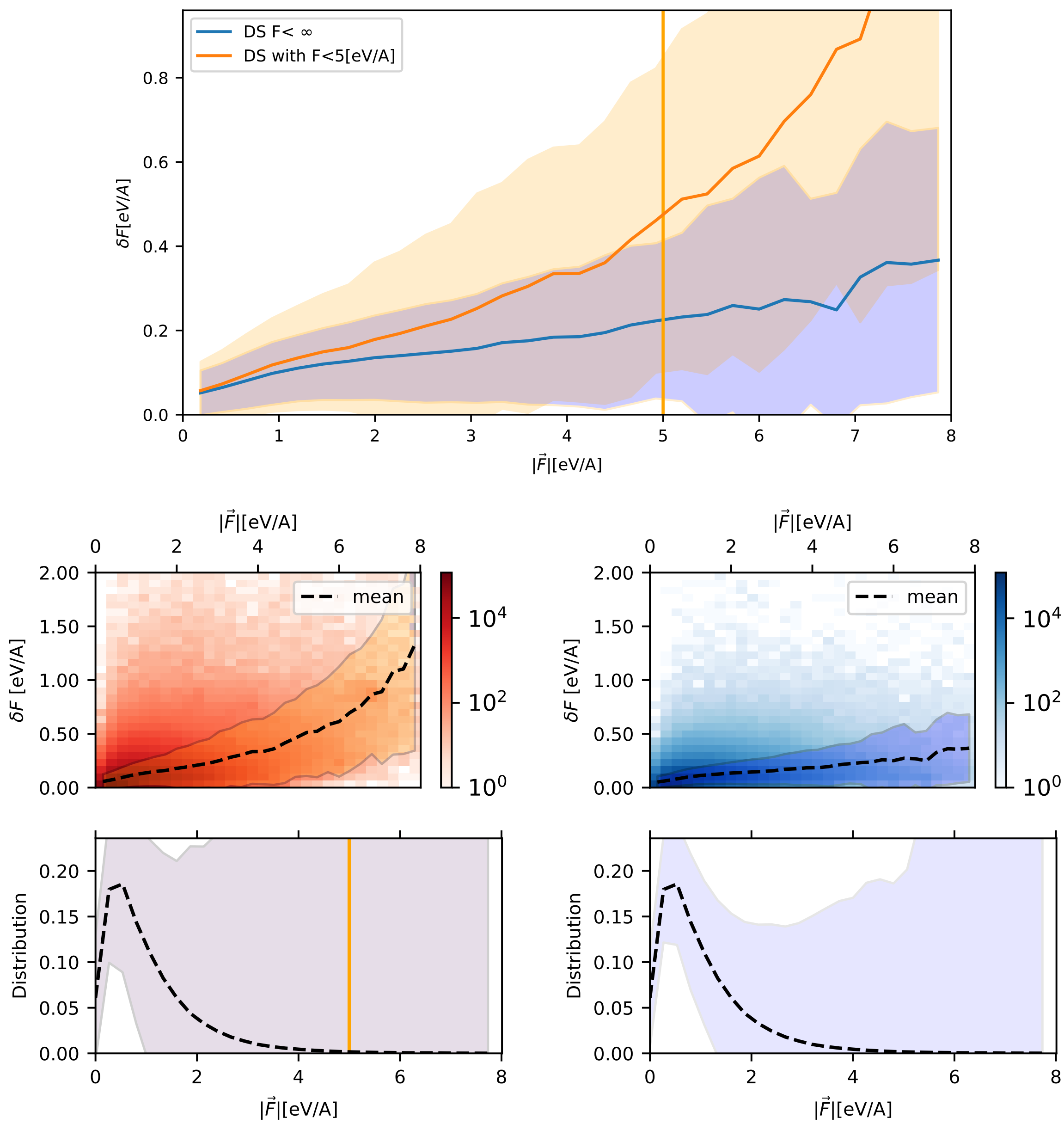


Figure SOI-3: The top panel of the graph illustrates the performance of two potentials: the orange curve represents the potential trained with a training set containing forces below 5eV/A, while the blue curve corresponds to a potential trained without restrictions on the magnitude of forces. Both potentials were trained with training set of identical size. Error bars represent the the standard deviation of $\delta F$ within each column bin. A vertical line is placed at $|\vec{F}| = 5\text{eV/A}$ to indicate the forces cutoff threshold. The lower panel displays the histogram of $\delta F$ as a function of force magnitude. Additionally, we provide a visualization of the forces distribution within our testing dataset. To aid interpretation, error bars are included to visually emphasize the standard deviation of $\delta F$ within each column bin. This illustrates into how the uncertainty of the forces correlates with force magnitudes.

## 4 Determination of the heat transfer coefficient

Figure SOI-4 shows the determination of the heat transfer coefficient $k$ for three differently sized gold nanoparticles on rutile $TiO_2$, corresponding to the three first rows in Table 3 of the main text.

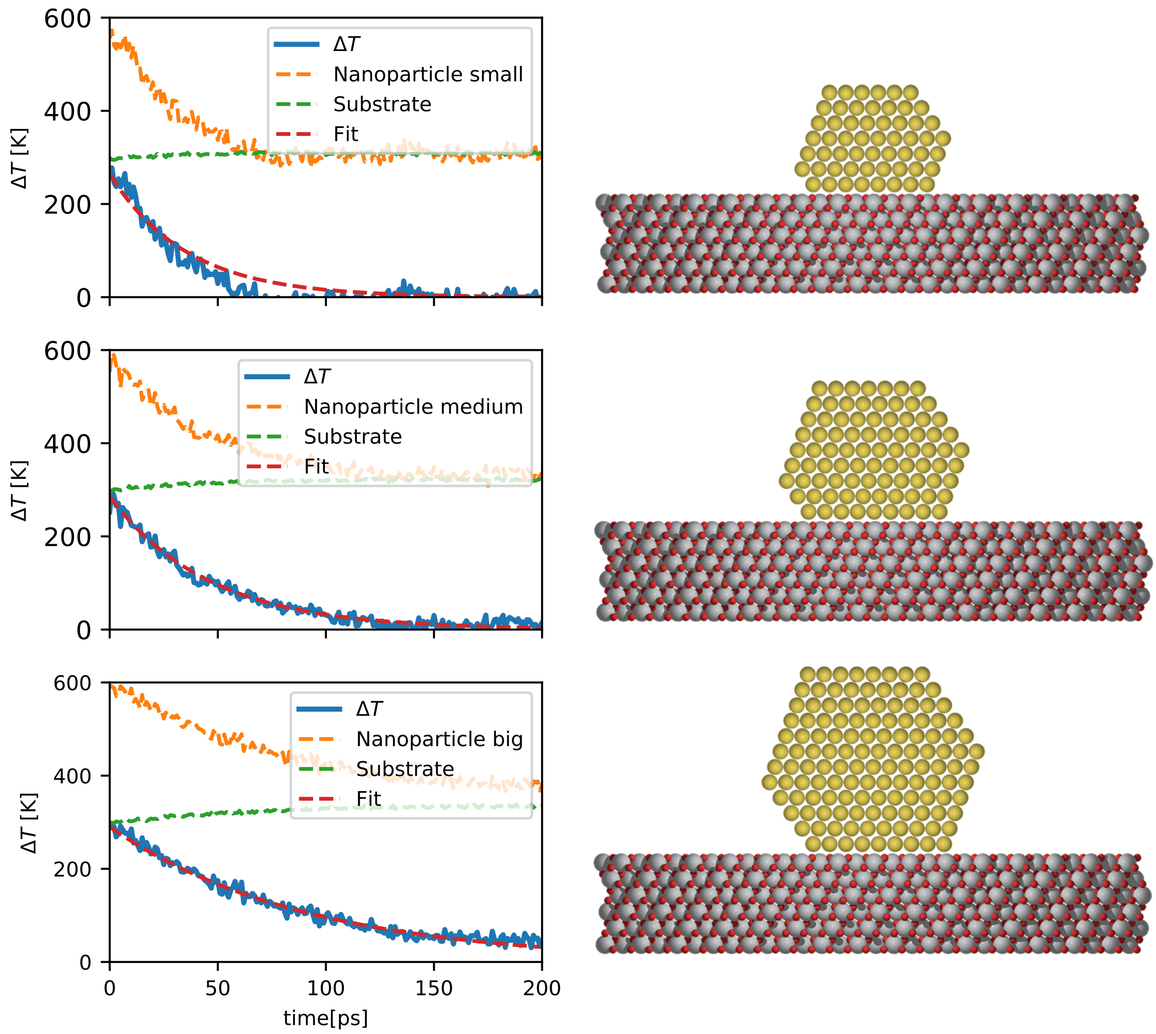


Figure SOI-4: Temperature fits of three different Au nanoparticles with different volume and contact area. The values for $k$ are $k = 1.08 \times 10^{-3}\,\mathrm{eV\,nm^{-2}\,ps^{-1}}$, $k = 1.12 \times 10^{-3}\,\mathrm{eV\,nm^{-2}\,ps^{-1}}$, and $k = 1.0 \times 10^{-3}\,\mathrm{eV\,nm^{-2}\,ps^{-1}}$ respectively.

## 5 Overview image of a sample

Figure SOI-5 shows an overview image of one of samples produced displaying gold nanoparticles on a hBN substrate, as described in the main text.

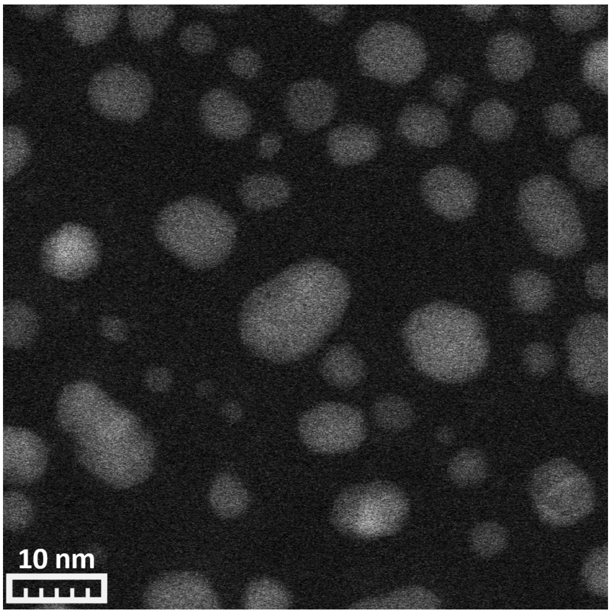


Figure SOI-5: STEM image of gold nanoparticles supported by hBN at 300keV

# 6 Additional determinations of the electron mean free path

The electron mean free path was determined from the most regularly shaped nanoparticles in Figure 7 in the main text. Similar results are found here from two additional nanoparticles at each beam energy, see Figure SOI-6.

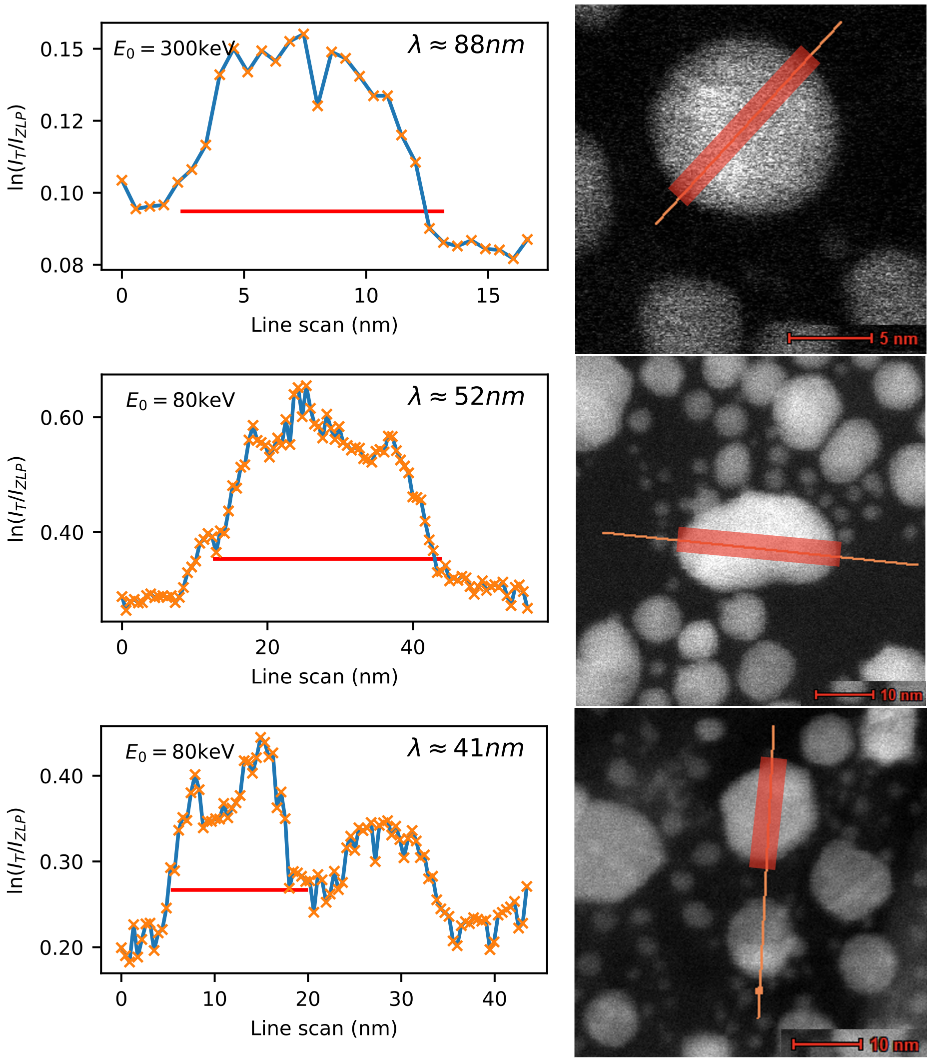


Figure SOI-6: Additional determination of the electron mean free path ($\lambda$) for nanoparticles of various shapes under different beam energies. The right column presents Scanning Transmission Electron Microscopy (STEM) images associated with the corresponding Electron Energy Loss Spectroscopy (EELS) spectra. In these images, the regions corresponding to the nanoparticles are delineated in red, indicating the specific areas analyzed in the line scans. Refer to figure 7 in the main text for methodology and comparative analysis.

# 7 Electron Energy Loss Spectrum

To determine the average energy loss per inelastic scattering event in Electron Energy Loss Spectroscopy (EELS), we analyze the inelastic low-loss region of the EELS spectrum, typically ranging from 5 to 110 eV and the Zero Loss Peak (ZLP) ranging from $-E_{th}$ to $-E_{th}$. The signal is treated as follows:

$$\text{Signal}(E) = \begin{cases} ZLP(E), & \text{if } -E_{th} < E < E_{th} \\ J(E), & \text{if } E_{th} < E < 110eV \end{cases}$$

Here, $E_{th}$ represents the elastic scattering threshold energy of the signal. This threshold is determined using the hyperspy package, which provides tools for EELS analysis. See Figure SOI-7.

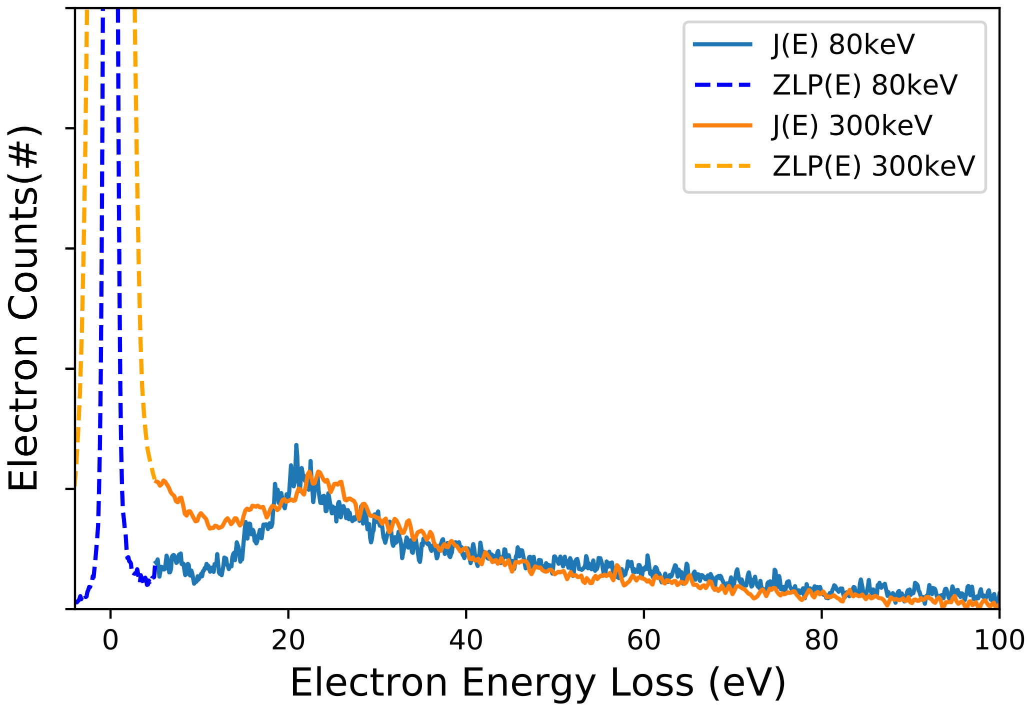


Figure SOI-7: Treatment of the signal, dotted lines are the ZLP region and solid lines are inelastic low-loss region of the EELS