Melting of FePt nanoparticles studied with DFT
Supplementary Material

Paweł T. Jochym, Jan Łażewski, and Przemysław Piekarz
Institute of Nuclear Physics, Polish Academy of Sciences, Radzikowskiego 152, 31–342 Cracow, Poland
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Structural animations are generated from the molecular dynamics using the following procedure:

- Find the best common scaling factor from the template structure to the optimized structure at low temperature.
- Fit the shift and rotation of the template structure to remove common movement of the system.
- Smooth the collective motions to remove only long-timescale motions from the trajectory.
- Adjust the position/rotation of each frame to match the template structure using the smoothed-out rotation and shift parameters.

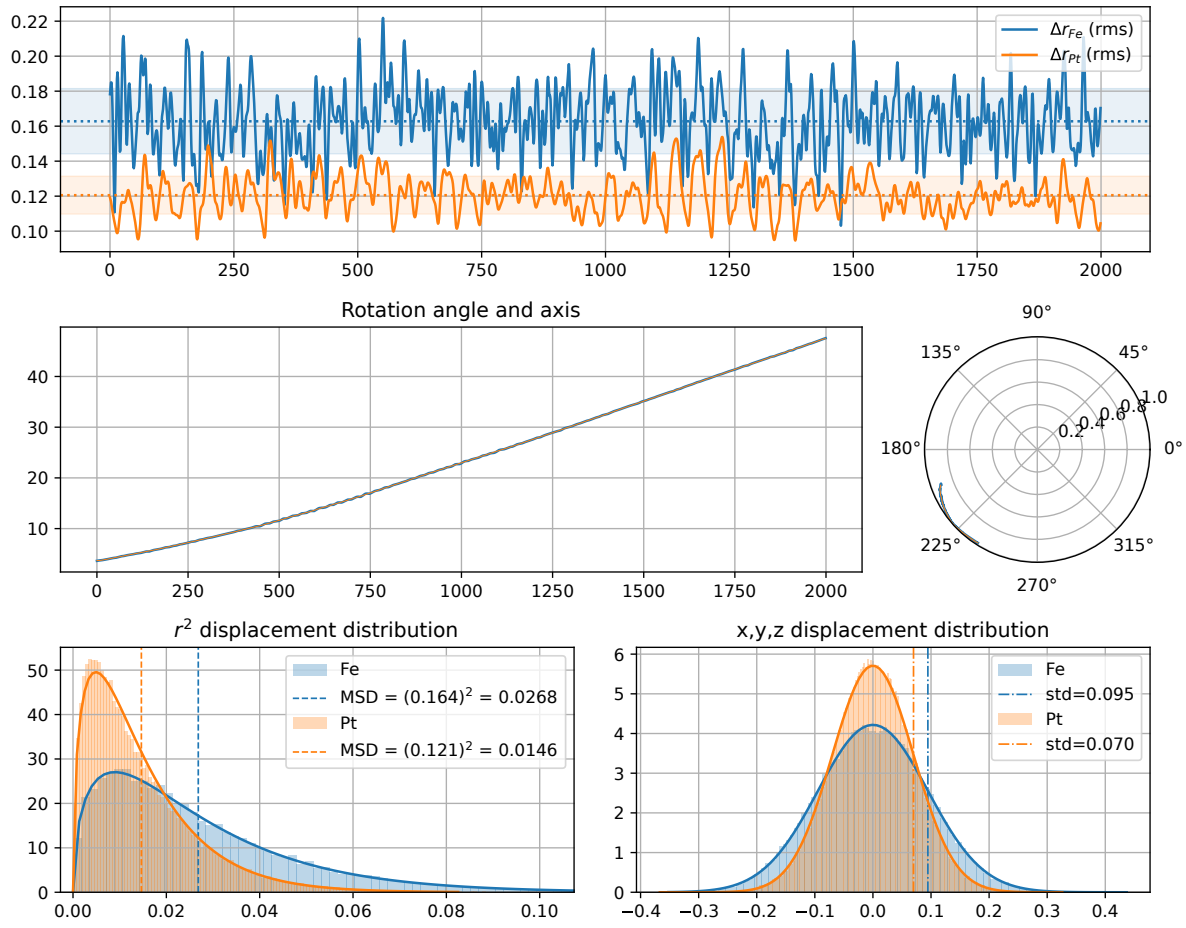

FIG. S1: Example fluctuations of atomic displacement in platinum-terminated icosahedral structure. The plot spans one 2000 steps segment at $T = 300$ K. The top plot shows the displacements of the atoms from the equilibrium positions over the time of the simulation. The plots in the middle show the rotation of the whole structure over the time of the simulation. The rotation is described as the rotation angle (left plot) and the direction of the rotation axis (right plot). The lower plots show the statistics of the square displacement (r^2, left plot) and single coordinate displacement for each element (right plot). The solid lines are fits to the statistics of the χ^2 with three degrees of freedom and normal distributions, respectively.

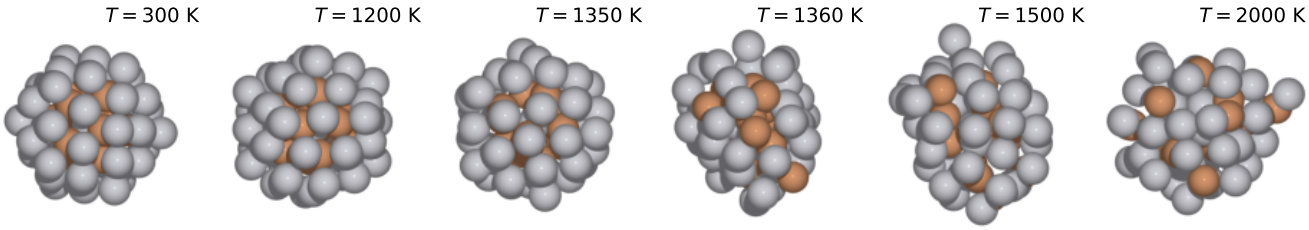

FIG. S2: Frames from the history of a melting of Pt-terminated structure. The temperatures have been selected to illustrate various stages of the process: stable structure (300 K, 1200 K), just below melting (1350 K), just above melting (1360 K), and fully melted (1500 K, 2000 K). At 2000 K the structure is probably on the brink of evaporation.

- Glue the normalized trajectory at the given temperature to the previous and next temperature in the sequence by linear combination of positions of corresponding atoms over the transition period of 10% of the length of the segment.

This procedure ensures the smooth movement of the particles in the animation while passing from one temperature to the next. It works well when the structure does not undergo any global reorganizations and atoms only vibrate around equilibrium positions. For the melted structure, this assumption no longer holds true and the large displacements of atoms changing their positions is visible as quick, collective motions over the transition periods. This non-physical effect is limited to the 10% of transition period. The remaining 90% of the trajectories are taken directly from the MD data and have only long-timescale drift and rotation removed to keep the physical motion of atoms, while making possible the visualization of the whole temperature scan (over 30 000 time steps) in a short animation. Fig. S3 shows example frames from these animations for all investigated structures. The full video files of the animations are available at following links:

- Platinum-terminated icosahedral structure ($Fe_{12}Pt_{43}$)
- Iron-terminated icosahedral structure ($Pt_{12}Fe_{43}$)
- Cuboctahedral structure ($Fe_{24}Pt_{31}$)

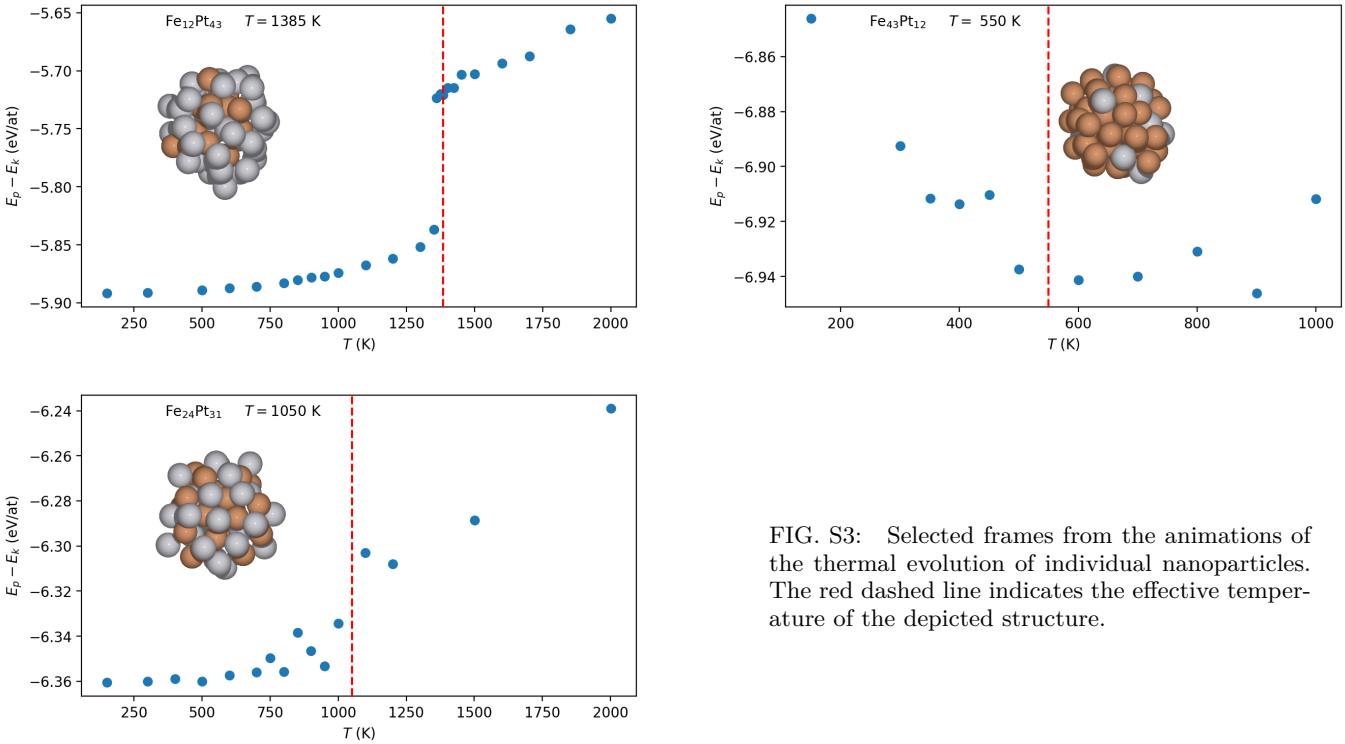

FIG. S3: Selected frames from the animations of the thermal evolution of individual nanoparticles. The red dashed line indicates the effective temperature of the depicted structure.