0.5 Supplementary

The the difference in the interatomic distance PCA is shown in Figure 10. For the middle energy tier, we list the ones that have the best maximum population for the tier in Figure 11/Figure 12 and we list some sample other middle tier minima in Figure 13/Figure 14. The difference in the atomic coordinate PCA are shown in Figure 11 and Figure 13, while the interatomic distance PCA are shown in Figure 12 and Figure 14. Finally, the highest energy tier that start with equal population are shown in Figure 9 and the energy tier just below them are shown in Figure 15. Note that the top high energy tier minima all relax exactly the same, probably since they have very similar energies and connectivities.

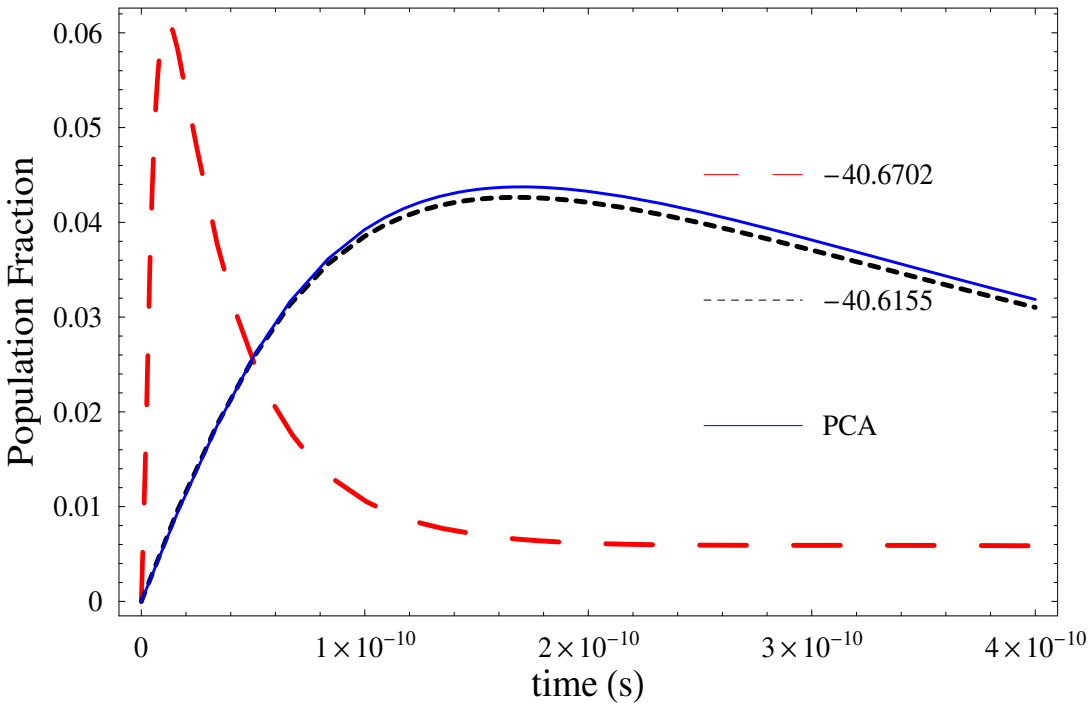

Figure 10: Relaxation curves of second most connected minima (second to the lowest energy tier). Interatomic PCA. Energies in ϵ.

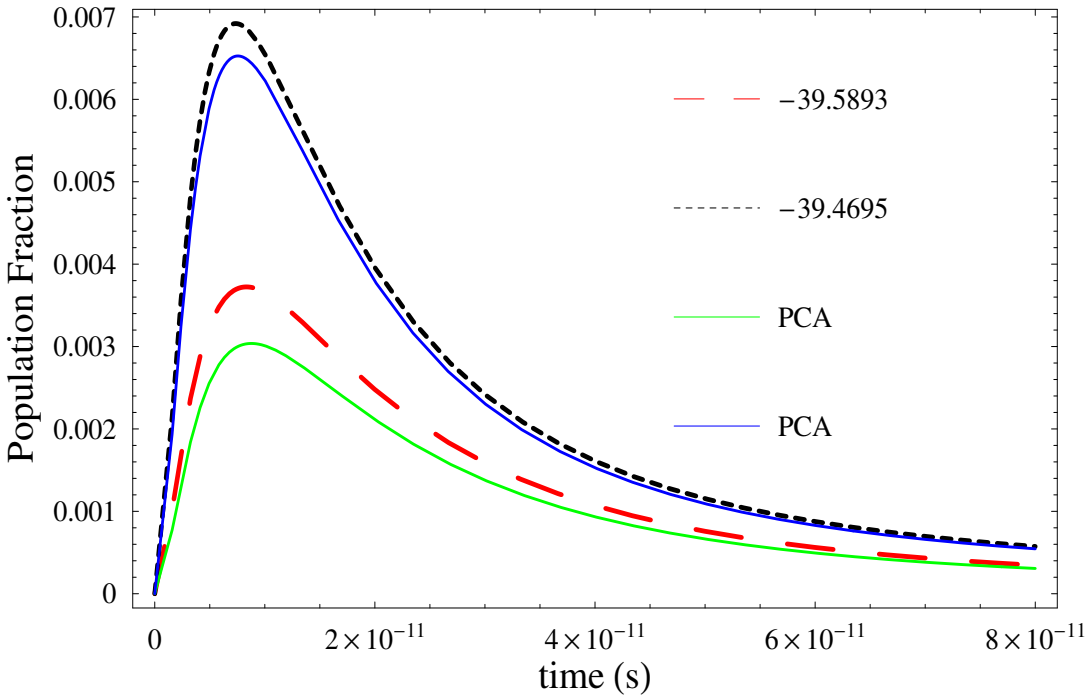

Figure 11: Relaxation curves of some middle energy tier minima which have better maximum population achieved than the rest of the middle tier. Atomic Coordinates PCA. Energies in ϵ.

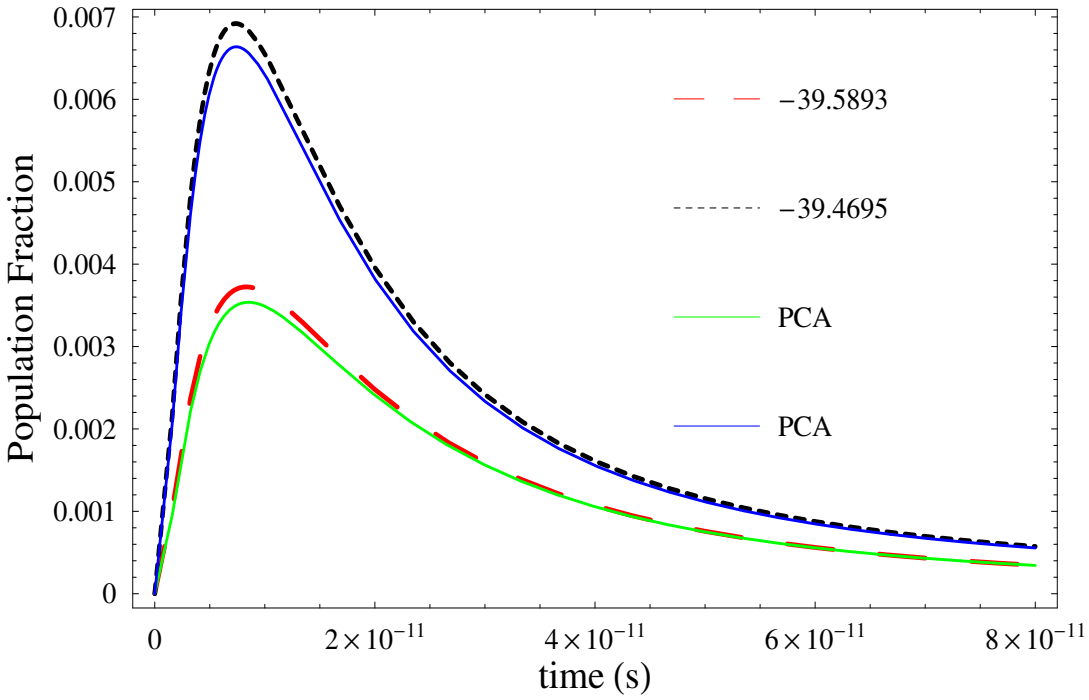

Figure 12: Relaxation curves of some middle energy tier minima which have better maximum population achieved than the rest of the middle tier. Interatomic PCA. Energies in ϵ.

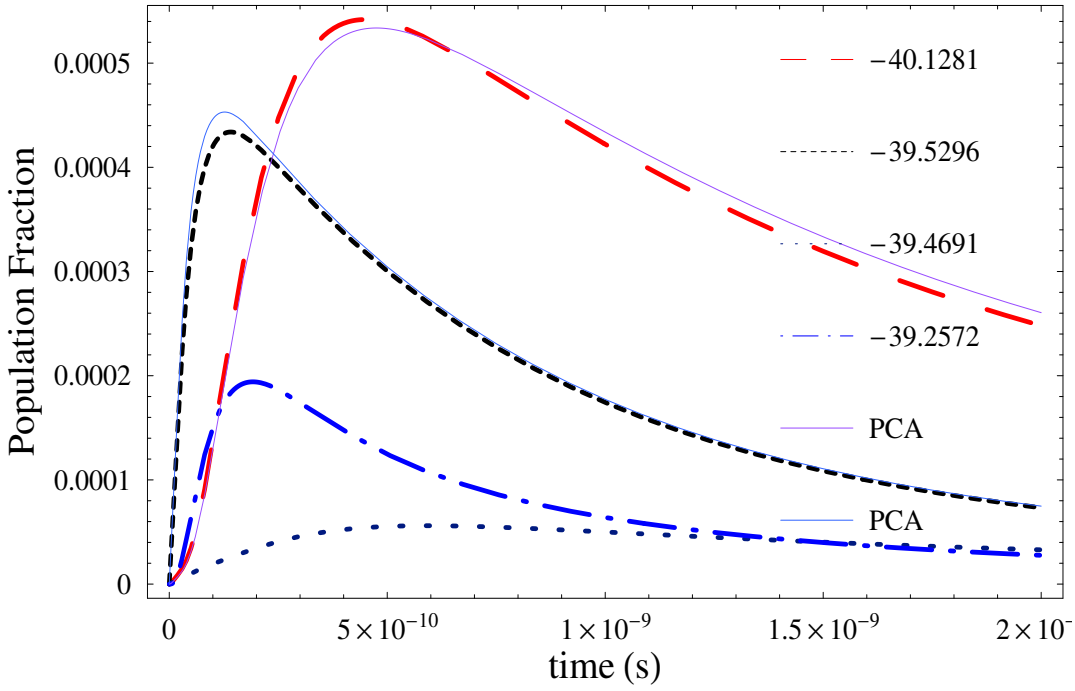

Figure 13: Relaxation curves of some middle energy tier minima. Atomic Coordinates PCA. Energies in ϵ.

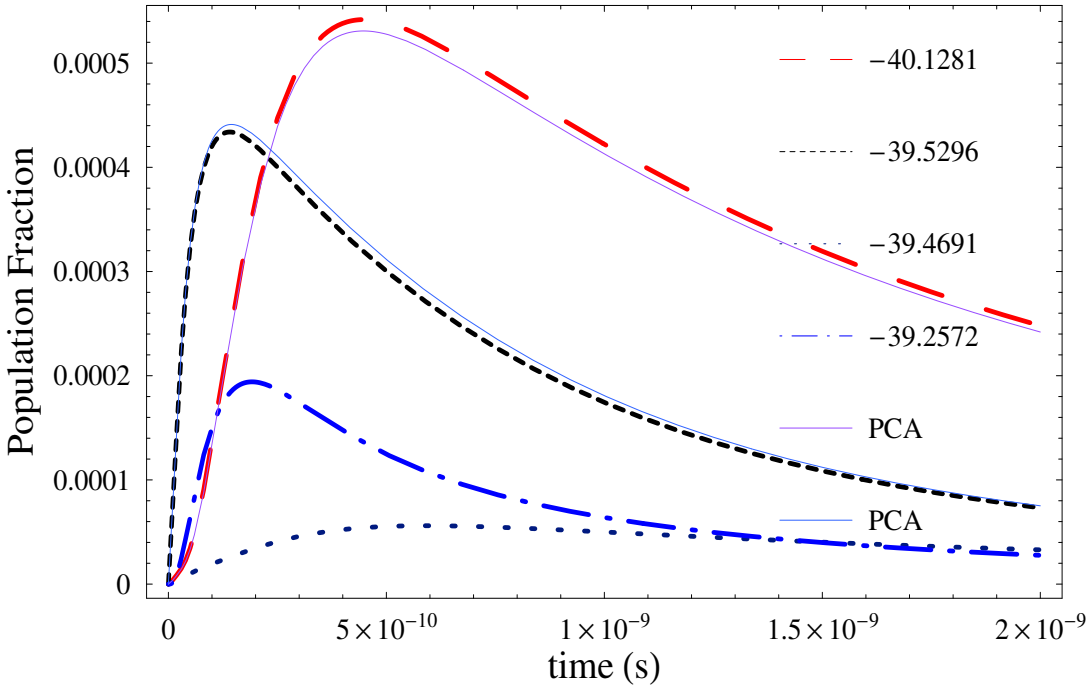

Figure 14: Relaxation curves of some middle energy tier minima. Interatomic PCA. Energies in ϵ.

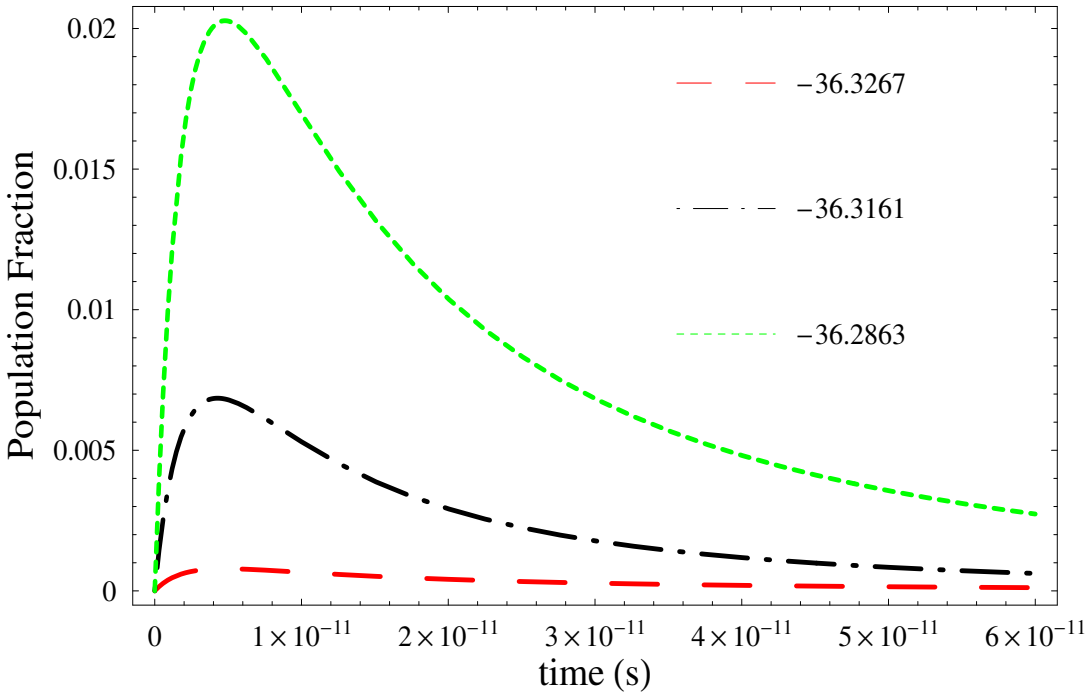

Figure 15: Some of the relaxation curves of the energy tier below the highest energy tier. Energies in ϵ.