

Supporting information:

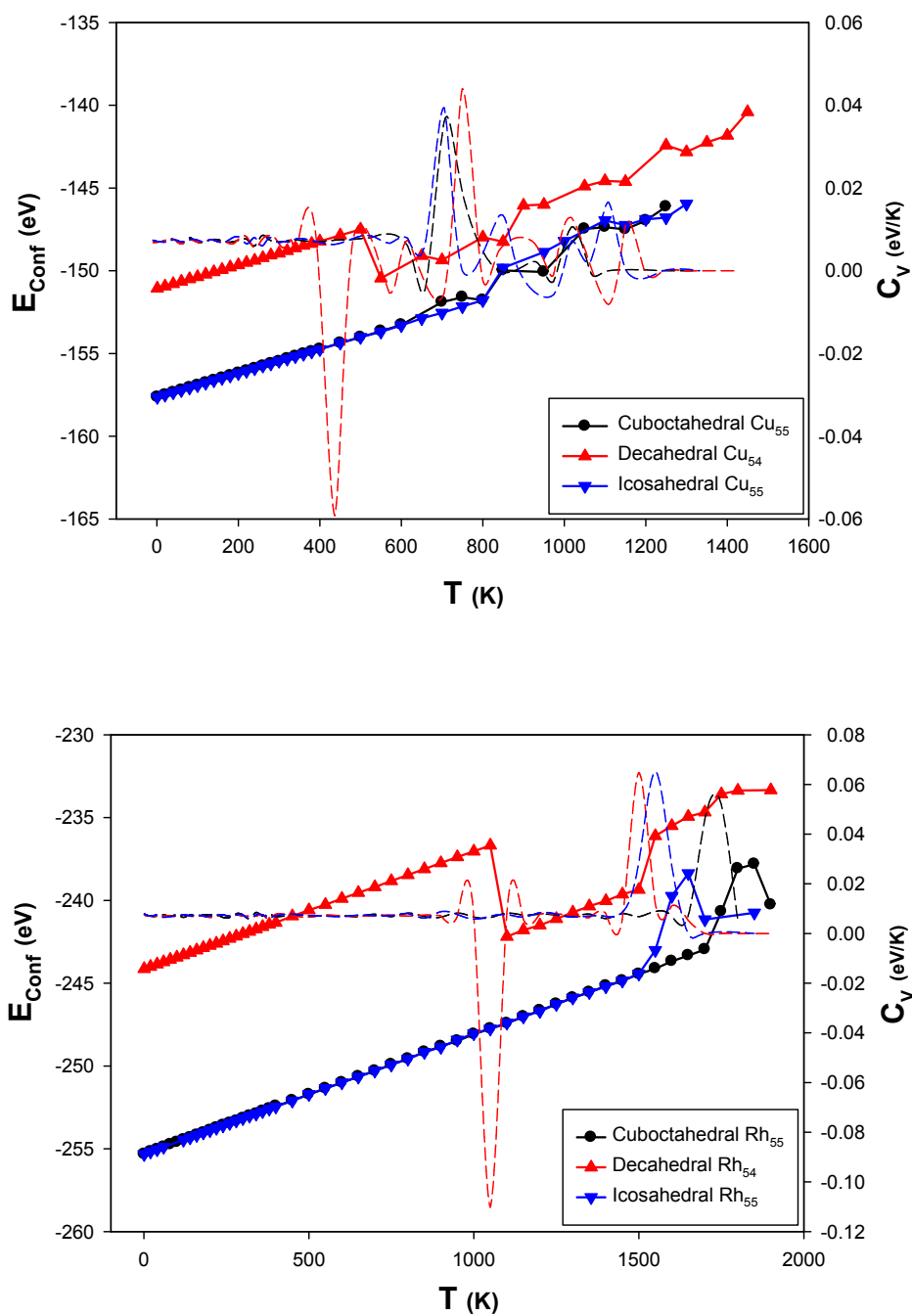
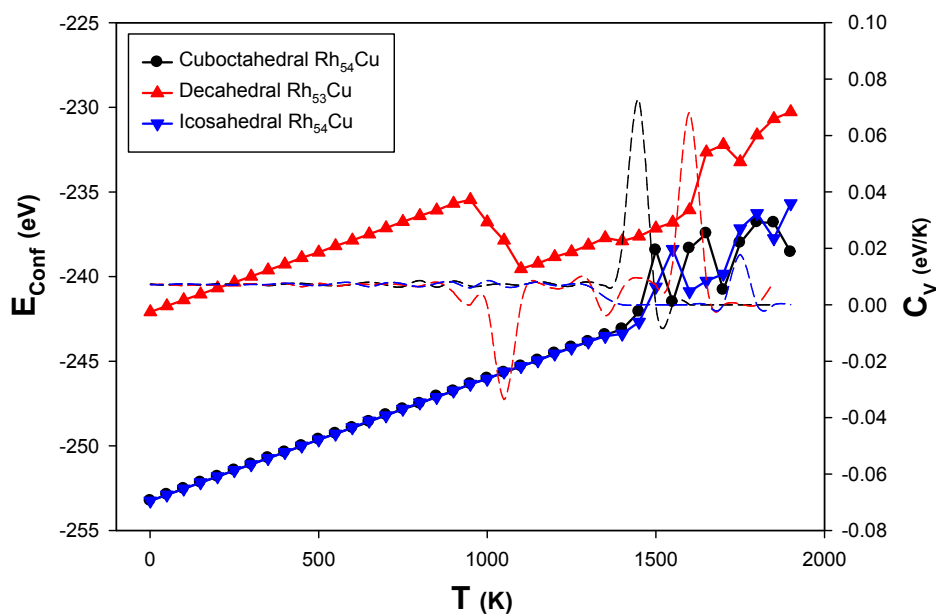
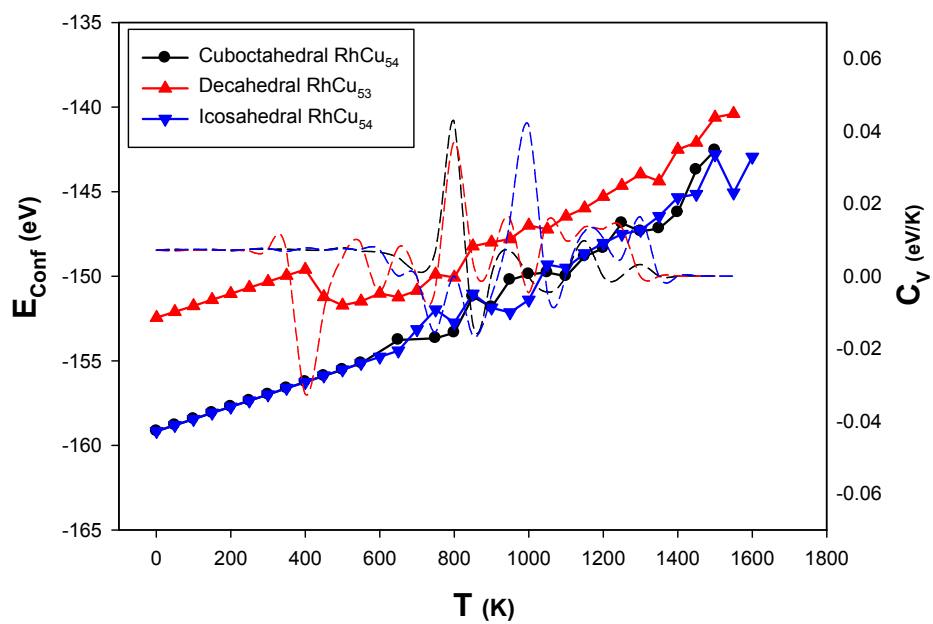
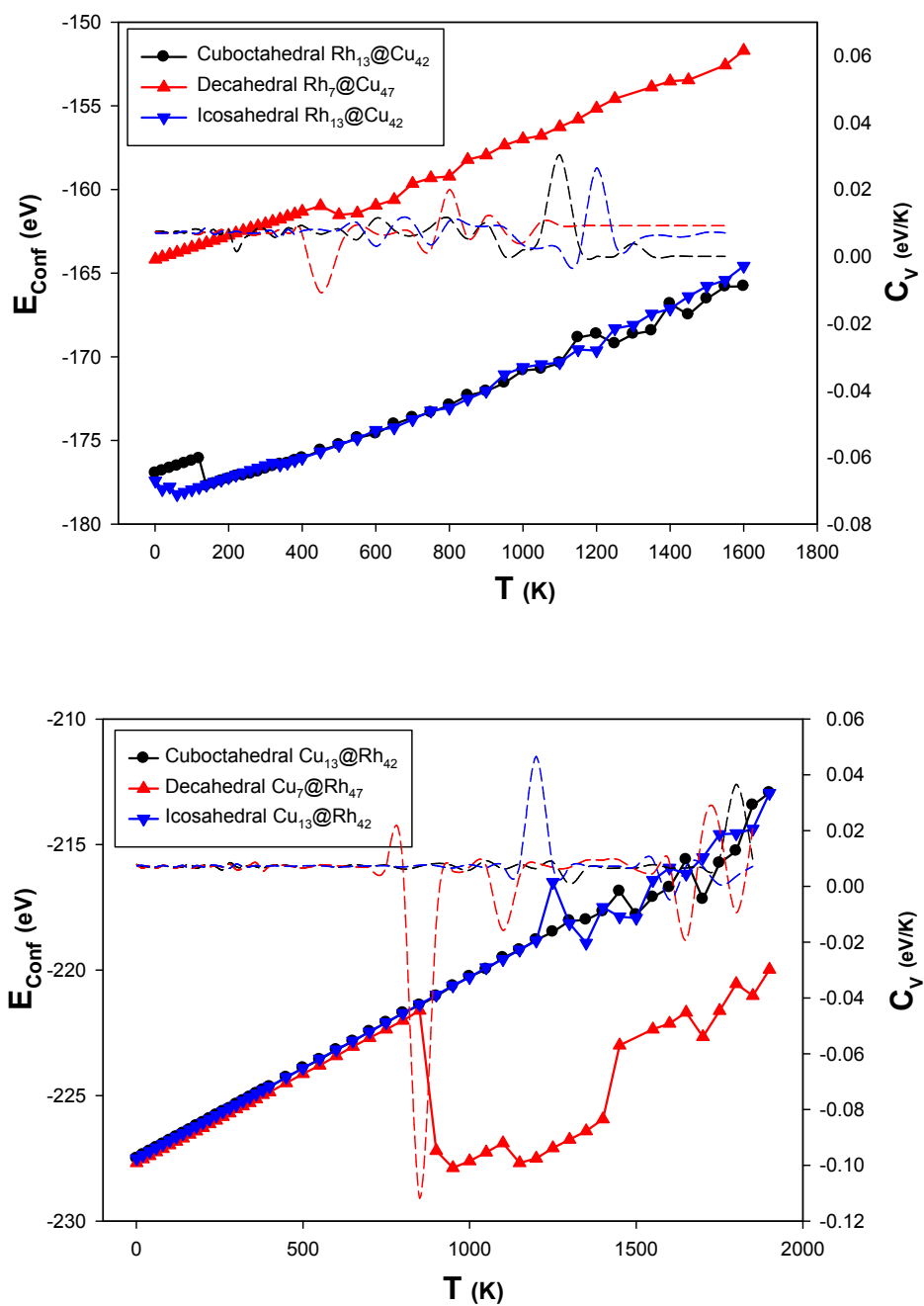


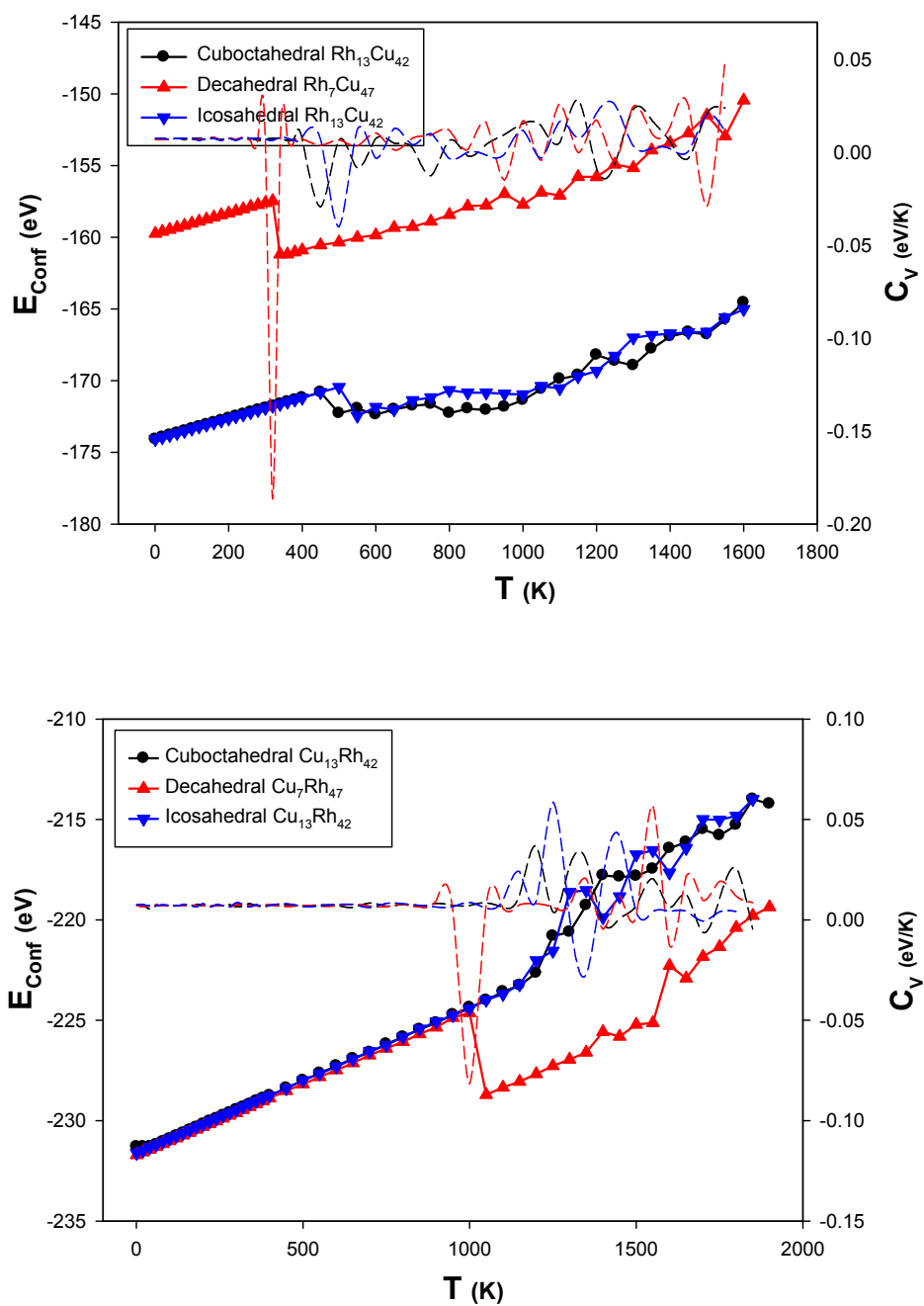
Fig. S1. The internal energy and heat capacity at constant volume for the pure copper and rhodium clusters in the three different structures.



**Fig. S2.** The internal energy and heat capacity at constant volume for the single dopant clusters in the three different structures.



**Fig. S3.** The internal energy and heat capacity at constant volume for the core@shell clusters in the three different structures.



**Fig. S4.** The internal energy and heat capacity at constant volume for the different clusters with the alloy arrangement in the three different structures.