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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.