Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information:

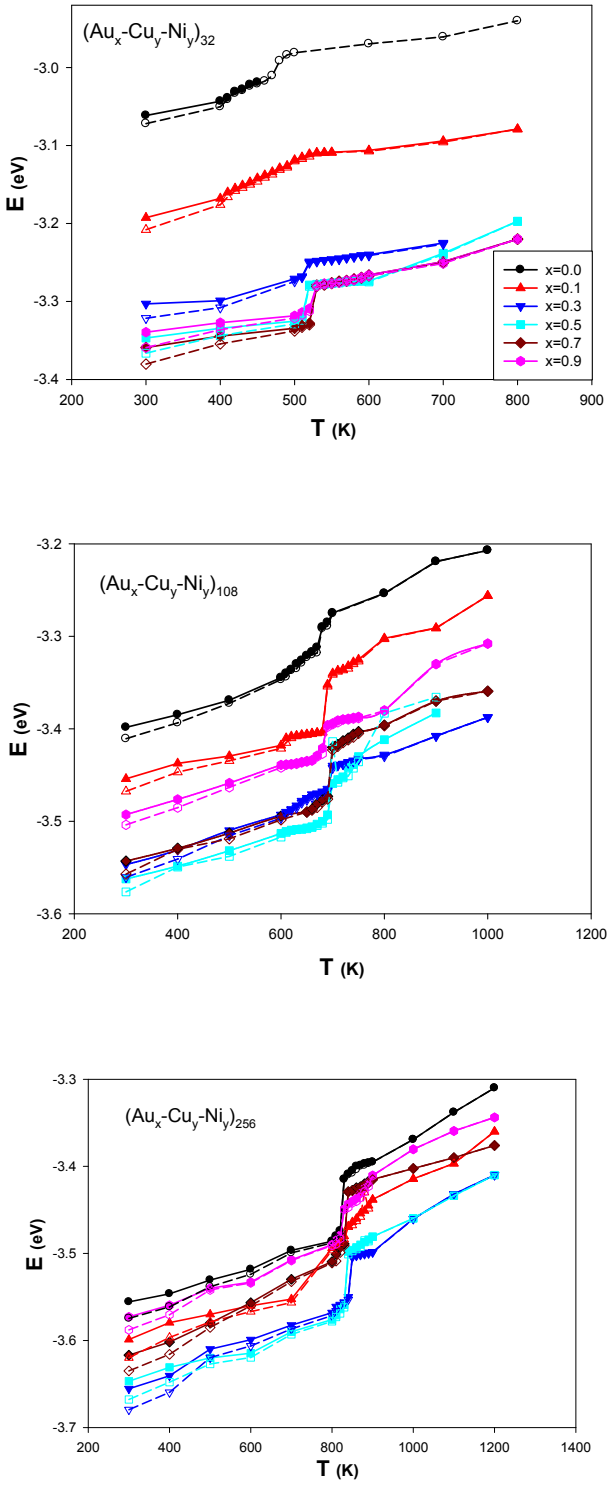

Fig. S1. The internal energies for the $(Au_x\text{-}Cu_y\text{-}Ni_y)_{N=32,108,256}$ nanoclusters with the different Au mole fractions at different temperatures in the heating and cooling processes.

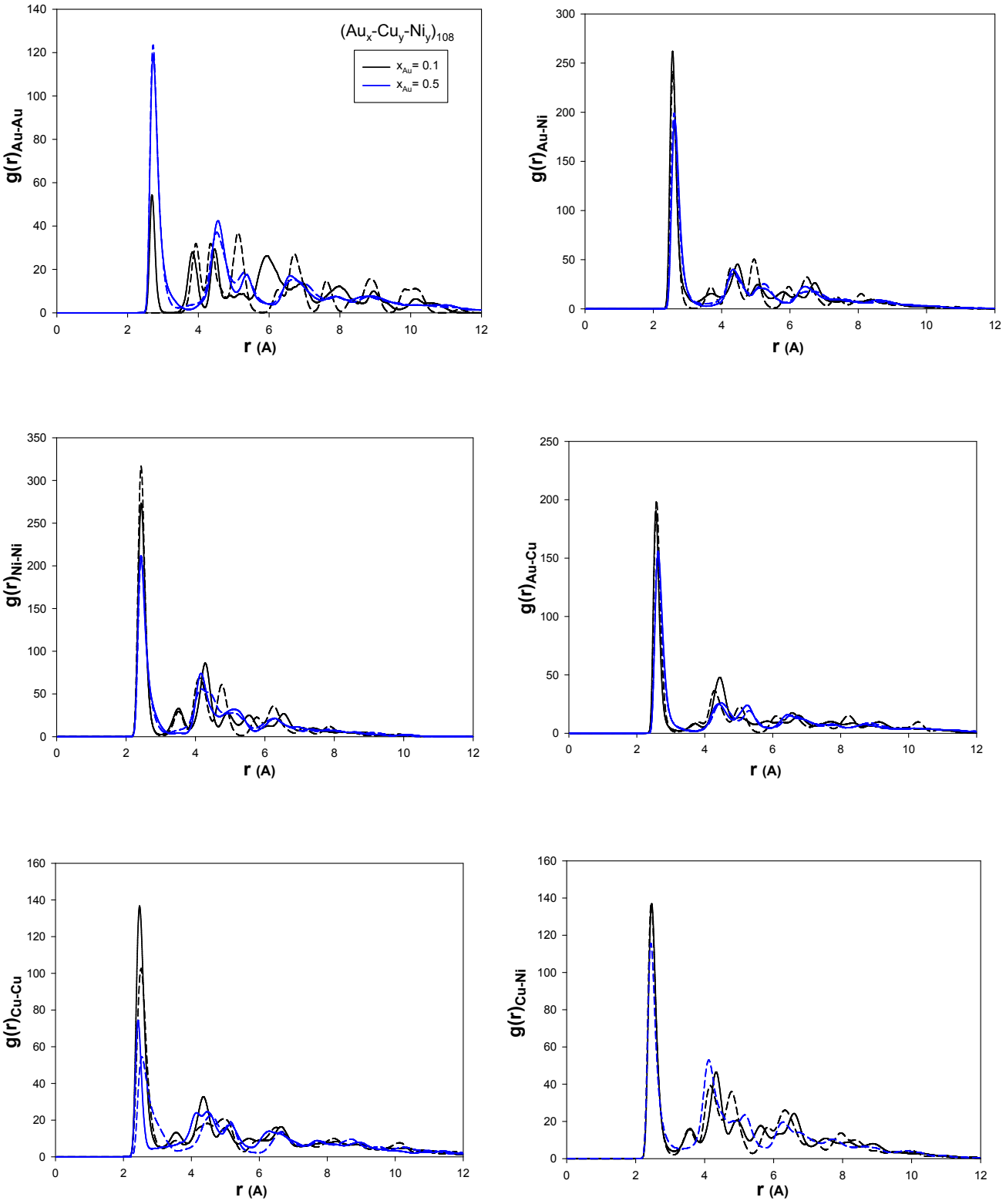

Fig. S2. The different RDFs for the $(Au_x\text{-}Cu_y\text{-}Ni_y)_{N=108}$nanoclusterat at initial at 300 K (the solid lines) and at 300 K after cooling process (the dashed lines) at different Au mole fractions.

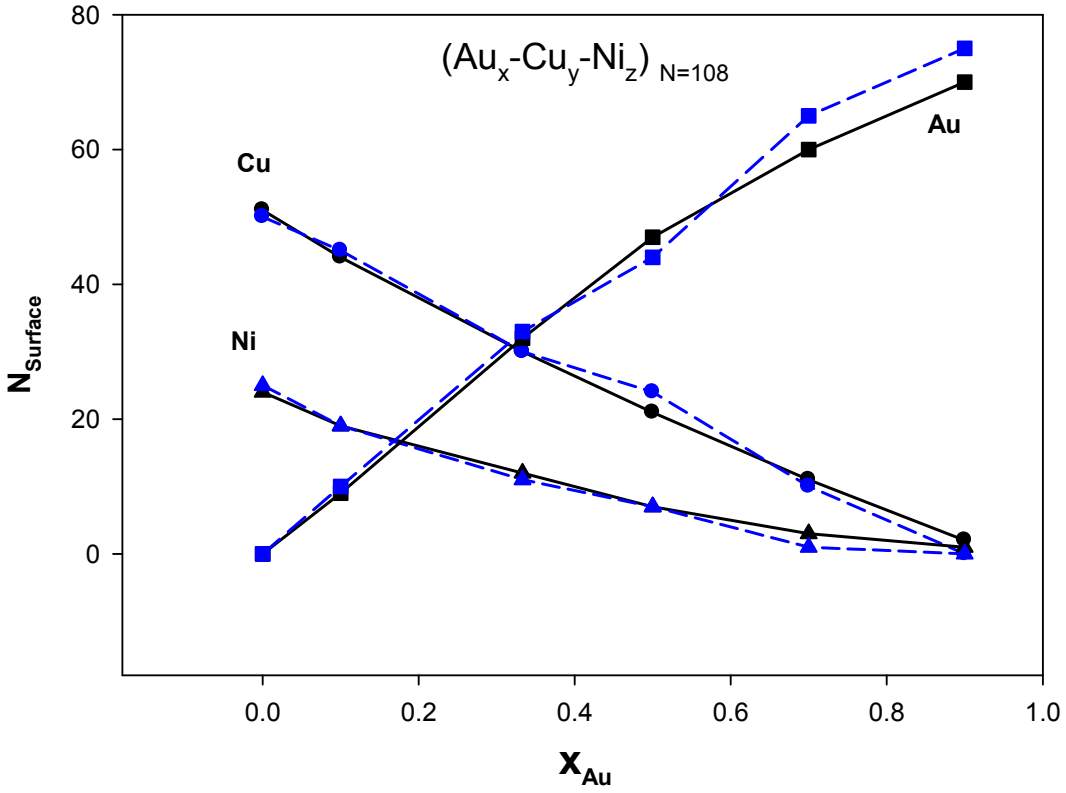

Fig. S3. The number of the Au, Ni, and Cu surface atoms in the $(Au_x\text{-}Cu_y\text{-}Ni_y)_{N=108}$ nanocluster at the initial at 300 K (the solid lines) and at 300 K after cooling process (the dashed lines) at the different Au mole fractions.

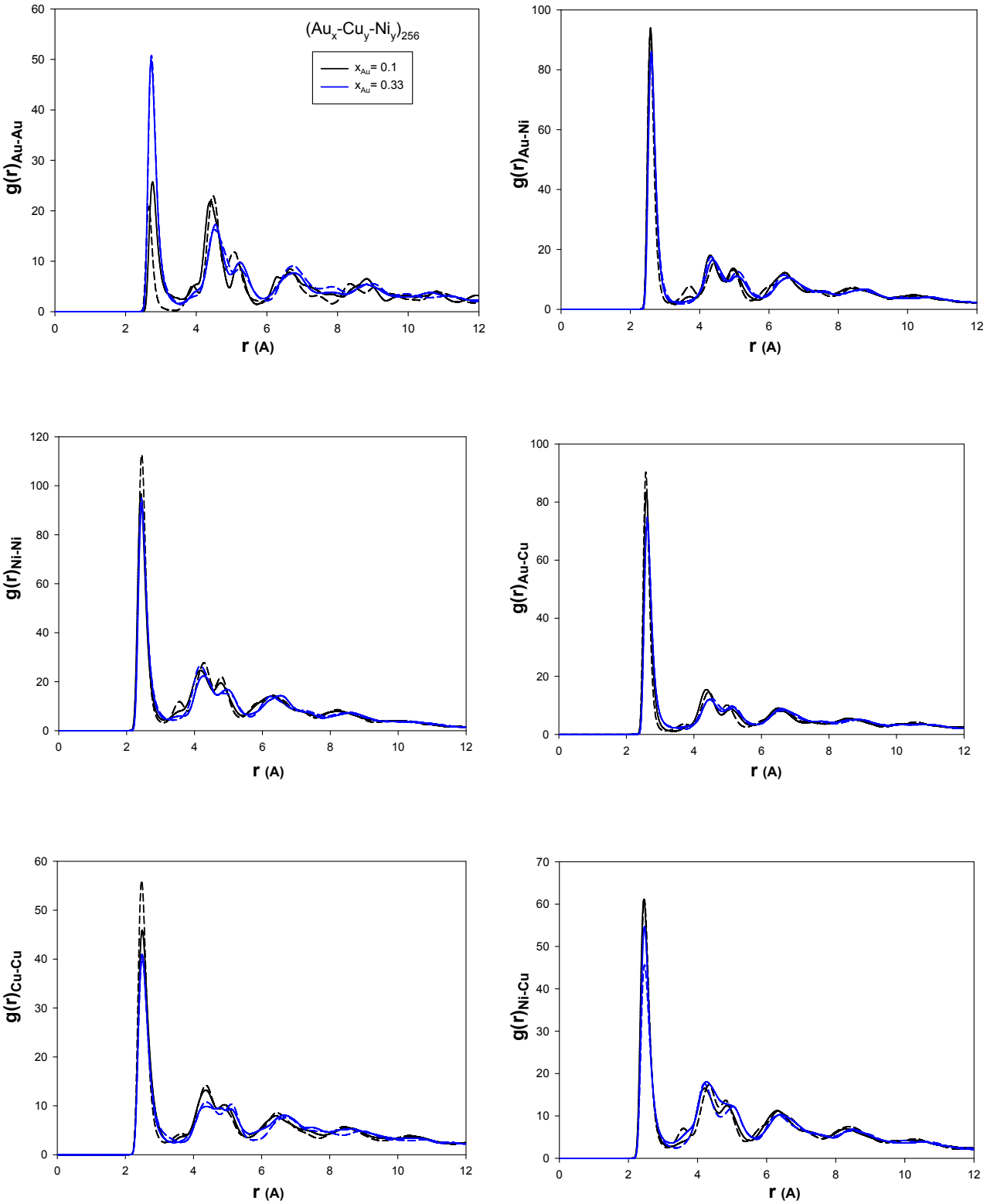

Fig. S4. The different RDFs for the $(Au_x\text{-}Cu_y\text{-}Ni_y)_{N=256}$nanocluster at initial at 300 K (the solid lines) and at 300 K after cooling process (the dashed lines) at different Au mole fractions.

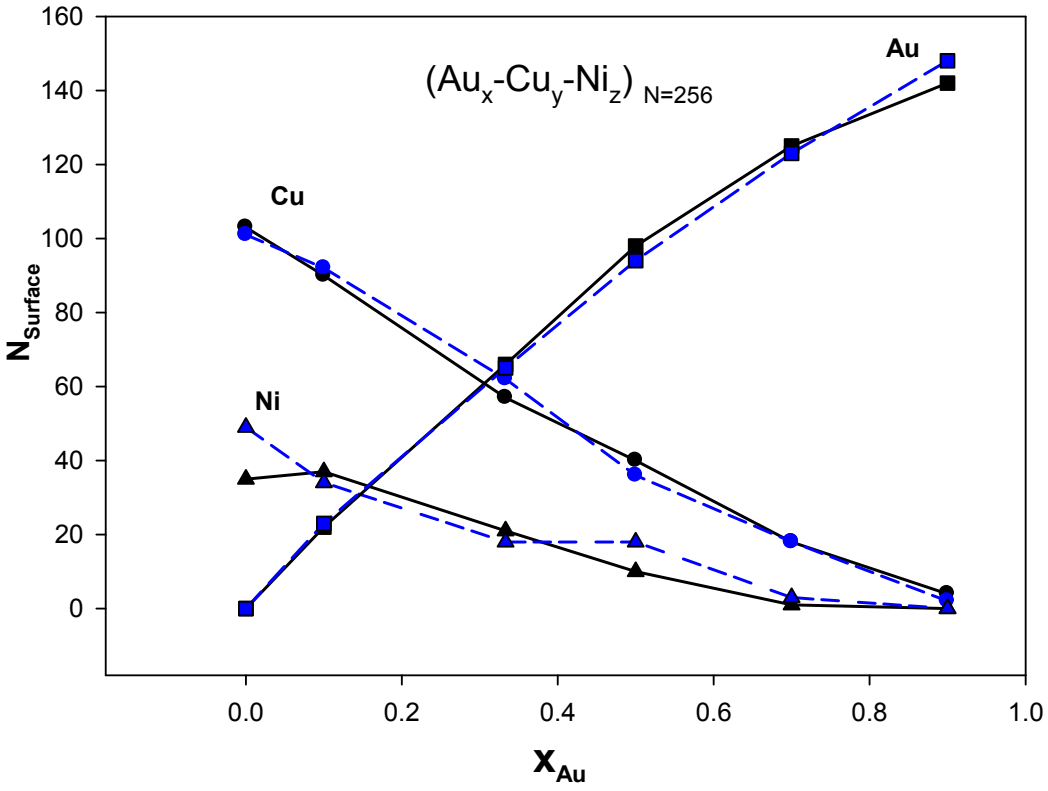

Fig. S5. The number of the Au, Ni, and Cu surface atoms in the $(Au_x\text{-}Cu_y\text{-}Ni_y)_{N=256}$ nanocluster at the initial at 300 K (the solid lines) and at 300 K after cooling process (the dashed lines) at the different Au mole fractions.