XXXII Panhellenic Conference on Solid State Physics and Materials Science
Conference Center "Carolos Papoulias", 18-21 September 2016, Ioannina, Greece

Structural, magnetic and electronic properties of CuFe nanoclusters by density functional theory calculations

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Abstract
Environmental sustainable magnetic nanoclusters and coatings have been proposed to meet specific technological demands (like superior magnetic properties) and being therefore promising for technological applications e.g. for the production of innovative nano-robotic platforms.
CuFe nanoclusters are very promising since they are free from hazardous and scarce raw elements. In this work we present density functional theory calculations on several $CuFe_x$ (x<10at%) nanoclusters aiming to reveal the relationship between the energetically favoured configuration and the magnetic moment. We have used the 13, 55, 147 and 309 icosahedral nanoclusters while the thin $CuFe_x$ coating on Cu(111) has been also studied for comparison reasons. We found that Fe atoms likes to aggregate inside the CuFe nanocluster revealing the pure Cu surface shell as the energetically favoured. The electronic density of states (EDOS) reveals the broad Cu bulk band from -5eV up to -0.5eV, mainly due to the Cu d electrons. In addition, the Fe atoms are mainly responsible for the spin majority and minority EDOS difference close to the fermi level introducing the magnetic character of the nanoclusters. Finally, the nanoclusters' magnetic moment is mainly due to the Fe d electron spin up – down mulliken charge population differences while it is found to be higher in the cases where the Fe atoms are segregated in the Cu surface cell. These results could be used for the design of environmental sustainable smart alloys with superior magnetic properties.

Acknowledgments: This work was supported by the SELECTA (No. 642642) H2020-MSCA-ITN-2014 project