

PERSONAL INFORMATION **Manoj Settem Narasimha**

WORK EXPERIENCE

- Feb 2021 – Present **Postdoctoral Researcher**
nanoCAFE Lab
Department of Mechanical and Aerospace Engineering
Sapienza University of Rome
- Finite-temperature structures of metal nanoclusters in the entire temperature range
 - Structure, energetics, and diffusion of Au clusters supported on graphene and graphite
 - Structural transitions in metal nanoclusters
- Jul 2013 – Dec 2015 **Instructor**
MAC Technologies (Education Company), Hyderabad, India
- Jul 2011 – Jun 2013 **Applications Engineer (Bright Field Optical Inspection)**
Applied Materials, Bangalore, India

EDUCATION

- 2017–2020 **PhD, Metallurgical & Materials Engineering**
Thesis Title: “Atomistic modelling of the structure and the stability of silver-copper nanoalloys”
Indian Institute of Technology Madras, Chennai, India
- 2009–2011 **Master of Technology, Metallurgical & Materials Engineering**
Indian Institute of Technology Kharagpur, Kharagpur, India
- 2004–2008 **Bachelor of Technology, Materials & Metallurgical Engineering**
Indian Institute of Technology Kanpur, Kanpur, India

PUBLICATIONS

- [1] **Manoj Settem**, Melisa M Gianetti, Roberto Guerra, Nicola Manini, Riccardo Ferrando, and Alberto Giacomello. “Gold Clusters on Graphene/Graphite—Structure and Energy Landscape”. In: **Small Science** 4 (2024), p. 2400078.
- [2] **Manoj Settem**, Mahabul Islam, and Ajeet K Srivastav. “Grain boundary junction disclinations in nanoparticles”. In: **Acta Materialia** 274 (2024), p. 120031.
- [3] Emanuele Telari, Antonio Tinti, **Manoj Settem**, Luca Maragliano, Riccardo Ferrando, and Alberto Giacomello. “Charting Nanocluster Structures via Convolutional Neural Networks”. In: **ACS Nano** 17 (2023), pp. 21287–21296.
- [4] **Manoj Settem**, Cesare Roncaglia, Riccardo Ferrando, and Alberto Giacomello. “Structural transformations in Cu, Ag, and Au metal nanoclusters”. In: **Journal of Chemical Physics** 159 (2023), p. 094303.
- [5] **Manoj Settem**, Riccardo Ferrando, and Alberto Giacomello. “Tempering of Au nanoclusters: capturing the temperature-dependent competition among structural motifs”. In: **Nanoscale** 14 (2022), pp. 939–952.
- [6] **Manoj Settem**, Pranav Kumar, Ilaksh Adlakha, and Anand K. Kanjarla. “Surface reconstruction in core@ shell nanoalloys: interplay between size and strain”. In: **Acta Materialia** 234 (2022), p. 118038.
- [7] **Manoj Settem**, Ajeet K. Srivastav, and Anand K. Kanjarla. “Understanding the strain-dependent structure of Cu nanocrystals in Ag–Cu nanoalloys”. In: **Physical Chemistry Chemical Physics** 23 (2021), pp. 26165–26177.

- [8] **Manoj Settem** and Anand Krishna Kanjarla. “Role of core-shell energetics on anti-Mackay, chiral stacking in AgCu nanoalloys and thermally induced transition to chiral stacking”. In: **Scientific Reports** 10 (2020), p. 3296.
- [9] **Manoj Settem** and Anand Krishna Kanjarla. “On the nature of the structural transitions between anti-Mackay stacking, chiral stacking and their thermal stability in AgCu nanoalloys”. In: **Computational Materials Science** 184 (2020), p. 109822.
- [10] **Manoj Settem**. “Novel structural motifs: chiral AgCu nanoalloys with chiral Cu core”. In: **Journal of Alloys and Compounds** 844 (2020), p. 155816.
- [11] **Manoj Settem**. “On the structural analysis of ordered B2 AlNi nanoparticles obtained using freezing simulations”. In: **Intermetallics** 106 (2019), pp. 115–123.
- [12] **Manoj Settem**, Mahabul Islam, and Anand Krishna Kanjarla. “On the effect of relative stabilities of FCC-like and HCP-like atoms on structure of FCC silver nanoclusters”. In: **Computational Materials Science** 148 (2018), pp. 266–271.
- [13] **Manoj Settem**, Piu Rajak, Mahabul Islam, and Somnath Bhattacharyya. “Influence of supporting amorphous carbon film thickness on measured strain variation within a nanoparticle”. In: **Nanoscale** 9 (2017), pp. 17054–17062.
- [14] Soumitra Chakraborty, **Manoj Settem**, and Sudhindra B. Sant. “Evolution of texture and nature of grain growth on annealing nanocrystalline Ni and Ni-18.5%Fe in air”. In: **Materials Express** 3 (2013), pp. 99–108.