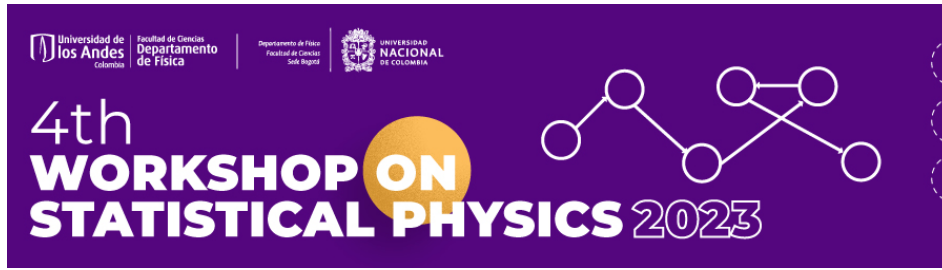


4th Workshop on Statistical Physics



Contribution ID: 54

Tipo: **Invited talk**

Determination of the free energy landscape of ultrasmall silver clusters with metadynamics and machine learning techniques

viernes, 6 de octubre de 2023 17:00 (20 minutos)

Ab initio metadynamics enables the extraction of free energy landscapes with the precision of first-principles electronic structure methods. We developed and used an interface between the PLUMED and ASE codes to estimate the free energy of Ag₅ and Ag₆ clusters at 10, 100, and 300 K with the radius of gyration and coordination number as collective variables [1]. We find that Ag₆ is the smallest silver cluster where entropic effects at room temperature increase the probability of the nonplanar isomer to a competitive state. To accelerate the determination of the free energy we currently use machine learning algorithms.

[1] J. Chem. Phys. 156, 154301 (2022)

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