

Abstract Submitted
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Unbiased search of minimal energy nanocluster structures¹ JOSÉ ROGAN, Universidad de Chile, GRISELDA GARCÍA, Universidad Católica de Chile, CLAUDIA LOYOLA, WALTER ORELLANA, Universidad de Chile, RICARDO RAMÍREZ, MIGUEL KIWI, Universidad Católica de Chile — A new strategy to find global minima is applied to the structure of metallic clusters. It consists in implementing a conformational space annealing (CSA) unbiased search in combination with many body phenomenological potential techniques to create a data bank of putative minima. Next, the clusters in this data bank are examined by first principle methods to obtain the minimum energy cluster. The scheme is successfully applied to magic number 13 atom clusters of rhodium, palladium and silver. Global minimum energy cluster structures not previously reported are found through our procedure.

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