Small Pd clusters: A comparison of phenomenological and ab initio approaches

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The lowest-energy structures of small Pd clusters (2?N?13) are computed by means of available phenomenological many-body potentials and by ab initio methods. The lowest-energy configuration is found by means of a genetic algorithm search. Satisfactory agreement between the results of the several methods implemented is achieved. Of special interest is the fact that all phenomenological potentials yield the same symmetry group for the lowest-energy cluster geometries, which moreover are identical with ab initio results. This constitutes an indication that the most common many-body empirical potentials can be trusted to yield reliable results.