Erratum: Global space-group optimization problem: Finding the stablest crystal structure without constraints [Phys. Rev. B 75, 104113 (2007)]

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Figure 5(b) in the published paper depicted erroneously not the lowest energy Au_8Pd_4 structure that we found, but another structure. The picture of the structure that has the lowest energy is now shown as Fig. 5(b) (No. 4820 in our list of fcc structures). We also provide below the atomic positions and unit-cell parameters of this (relaxed) structure (Table I):

Table I. Space Group: C*mcm* (No. 63 of the International Tables of Crystallography). Unit-cell parameters: a=3.9670 Å, b=6.3189 Å, c=8.0040 Å, α=90°, β=90°, γ=71.7054°. Atomic positions (fractional coordinates):

Au(1): (0.334408, 0.331184, 0.998269)
Au(2): (0.665592, 0.668816, 0.001731)
Au(3): (0.502058, 0.995884, 0.250000)
Au(4): (0.834174, 0.331652, 0.250000)
Au(5): (0.334408, 0.331184, 0.501731)
Au(6): (0.665592, 0.668816, 0.498269)
Au(7): (0.497942, 0.004116, 0.750000)
Au(8): (0.165826, 0.668348, 0.750000)
Pd(1): (0.000000, 0.000000, 0.000000)
Pd(2): (0.166849, 0.666302, 0.250000)
Pd(3): (0.000000, 0.000000, 0.500000)
Pd(4): (0.833151, 0.333698, 0.750000)

Furthermore, it has been drawn to our attention that the manner in which the abstract of our paper discusses previous publications might appear not to give suitable acknowledgment to work by Oganov and Glass (Refs. 34 and 35 in our paper), or to work by Abraham and Probert (Ref. 13 in our paper), published in the months prior to the submission of our manuscript. The main text of our published paper has correctly described and acknowledged previous applications of evolutionary algorithms to crystal geometry optimization, stating: "This method is based on an evolutionary algorithm,[31] following earlier works of Deaven and Ho,[32] Abraham and Probert,[33] Oganov *et al.*,[34] and Oganov and Glass.[35]" (all reference numbers from our published paper). To establish a clear and consistent relation between what is said in the main text and in the *abstract*, the fifth sentence of the abstract is amended to the following: "We present here our own implementation of an approach to the global space-group optimization (GSGO) problem, i.e., the problem of predicting both the lattice structure and the atomic configuration of a crystalline solid." The last sentence of the *abstract* is amended to the following: "Along with the previous work on global optimization by Deaven and Ho [Phys. Rev. Lett. **75**, 288 (1995)] applying genetic algorithms to clusters, and its generalization to solids by Abraham and Probert [Phys. Rev. B **73**, 224104 (2006)], Oganov, Glass, and Ono [Earth Planet. Sci. Lett. **241**, 95 (2006)], and Oganov and Glass [J. Chem. Phys. **124**, 244704 (2006)], this evolutionary-algorithm approach to GSGO opens the way to predicting unsuspected structures by direct optimization."

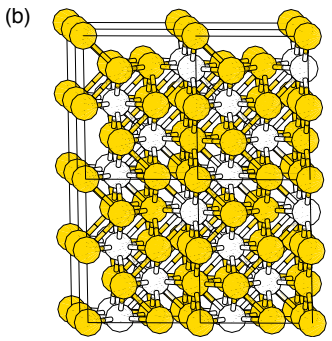

FIG. 5. (Color online) Ground-state structure of Au8Pd4 found by GSGO (No. 4820 in our list of fcc crystal structures).

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