Random structure generator with fixed environment

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Crystal structure generators existing today do not allow adding and fixing known structural information (i.e., environment). Solution of this problem is necessary in cases when the positions of some atoms can be determined using experimental techniques. In this work we present a new random structure generator that allows one to specify known structural information such as the size of a cell and the position of certain atoms or molecules in it. We illustrate this method by applications to hydrides with fixed positions of heavy atoms at different pressures and evaluate the structural diversity of the obtained crystals. Generated structures were used as seeds in the evolutionary algorithm USPEX [1], where VASP relaxation was performed. The found stable phases of lanthanum, uranium, and sulfur hydrides are in agreement with the experimental results from [2], [3] and [4] respectively. Also, using the approach, we searched for a stable experimental phase of magnesium hydride. We also found stable structures of $CL_{-}20 \cdot N_2O$ molecular crystal, which can be used as energetic materials.

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