Big bang methodology applied to atomic clusters

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An implementation of a novel strategy for cluster geometry optimization, using a stochastic method, is applied. This algorithm is based on the spirit of Big Bang theory. The strategy consists on a three-step procedure; a semiempirical optimization of the 1000n super compressed starting geometries, followed by two DFT optimizations of the resulting structures. The methodology is applied to the study of alkali metal clusters (Lin with 3 ? n ? 20, Nan with 3 ? n ? 13, and Kn with 3 ? n ? 10) structures and properties. With this new technique, we were able to find new isomers. The structures of alkali clusters show a large number of pentagonal pyramids and tetrahedral subunits. Most important electronic properties have been discussed and compared with different calculations and experimental data.