# Basin Hopping

What are the principles of basin hopping?

Basin Hopping is an algorithm that finds the global minimum for the Lennard-Jones (LJ) potential energy surface for clusters of atoms. Like many other Global Optimization algorithms, Basin Hopping attempts to find the points or energy in the system in which the gradient(s) is equal to zero. Running through all possible values of a function may be prohibitively expensive even with todays computational abilities, thus basin hopping attempts to alter the the Energy Potential surface into a series of minima step functions. This does not alter any local minima, but saves computation time by eliminating points for which the algorithm needs to cycle through. Using Monte Carlo simulation at a constant reduced temperature, the energy landscape is explored. At each step, all coordinates were displaced by a random number in the range [-1,1] times the step size, which was adjusted to give an acceptance of 0.5. The transformed surface allows for relatively large step sizes, which reduces the total number of iterations required. For each cluster in the range considered, seven separate runs are conducted. Five of which consists of 5000 Monte Carlo steps stating from different randomly generated configurations of atoms confined to a sphere of radius 5.5 reduced units. The subsequent geometry optimizations employs a container of radius one plus the value required to contain the same volume per atom. The Monte Carlo cutoff is the RMS of the gradient less than 0.01 in reduced units. The lowest energy structures obtained during the simulations are saved and re-optimized with tolerances of 10^-4 and 10^-9 for the RMS force and energy difference. The final energies are accurate to about six decimal places. After all the energies are found then each are compared with the smallest being the global minimum.

Choose three numbers to run the basin hopping?

n=13, n=15, n=19

what are the parameters which could lead to the global minimum?

The parameters that could lead to finding the global minima are the energy function of the lenard jones potential energy surface, the radii of the lenard jones potential, the step size of the monte carlo simulation. The well depth and well depth are also factors.