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A divide and conquer method for Bader decomposition JUN-ICHI HOSHINO, KAZUO TSUMURAYA, Meiji University — The ionicity of atoms in crystals or molecules is a measure of the bonding states among the atoms. There have been several methods to evaluate the electron charges that belong to each atom. Bader analysis is a direct method and divides up into atomic regions where the dividing surfaces are at a minimum in the charge density. [1] The algorithm, however, has computational difficulties to find the critical points for complex circumstance of atoms. A Henkelmans algorithm [2] is free of the points, assign each point on a regular grid to one of the regions by following a steepest ascent (SA) method contrary to the Baders steepest descent (SD) algorithm. We have found the SA method separates the regions more precisely than the SD method, although they are reverse relation. The SA method however requires much memory capacity for all-electron densities which are oscillating in the core regions. We implement a divide and conquer method to calculate the core region separately from the other region, assess the proposed method, and compare it with the Henkelmans decomposition.

1. R.Bader, Atoms in Molecules:A Quantum Theory, Oxford,1990.

2. G.Henkelman,et al., Comp.Mater.Sci.(in press)

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