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Evaluation of Magnetic Moments using Bader Analysis TOMOHARU SHIKAUCHI, KAZUO TSUMURAYA, Meiji University, Japan — Evaluation of the magnetic moments in solids is crucial in the computational physics. The moments have been calculated by an atomic sphere approximation or a Voronoi polyhedron approximation. There has been a method to partition the space with the minimum electron charge density surface, called zero flux planes, around each atom. The space is called Bader region. We apply the method to calculate the local magnetic moments of each atom depending on their circumstance using the first principle electronic structure calculation. We obtain the moments from the Bader charges using the up-spin charge and the down-spin charges. We apply the validity of this scheme to the analyses of the spin moments in Fe-N compounds, fcc Fe, and bcc Fe crystals and compare them with the experimental values. For Fe_4N, the difference of the moments between Fe(I) and Fe(II) atoms has been larger than that of the Voronoi method and is better agreement with the experimental values than the Voronoi method.

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