

Total-Energy and Electronic Structure in Magnetism

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The field of magnetism, especially understanding of itinerant-electron magnetism, has greatly prospered from *ab initio* electronic-structure calculations and the determination of the total energy. This is not supposed to be a complete overview, but some key-points will be made, chosen quite subjectively to fit the occasion. Beginning roughly in the seventies, for example, the foundation was laid by Terakura for the understanding of the famous Slater-Pauling curve, work that was in the eighties completed by him and collaborators at the IBM-Thomas J. Watson research center. There he also tackled transition-metal oxides resulting in a paper that initially caused quite a stir in the community. More important, however, it helped to initiate a great number of essential improvements in the electronic structure methodology as can be seen by looking at recent work by Terakura and his group on Mott insulators, Manganates and many other fascinating topics.