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Electronic Structure of Isolated Guest Atoms

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Taking advantage of its unique supply of radioactive isotopes, groups of experimentalists apply nuclear techniques to investigate the properties of solids, surfaces, and soft matter at ISOLDE. The methods of choice are Moessbauer, perturbed angular correlation, and nuclear magnetic resonance spectroscopies. In addition to existing facilities, a set-up for the beta-NMR-technique has been transferred to ISOLDE which will expand the range of available isotopes by using tilted foils for polarising post-accelerated radioactive ion beams.

With the advent of powerful computer codes, the interpretation of the experimental results has been based on unifying principles. For example, the magnetic hyperfine fields and the electric field gradients of Cd guest atoms on ferromagnetic nickel, which have been measured by the "ASPIC" group, can be related to the partial wave scattering of electrons on the impurity potentials. For sp-elements in particular, magnetic fields are dominated by a polarisation in the local s-band, while field gradients are derived from an asymmetry in the population of p-sublevels.

In the wake of extended simulations similar electronic configurations have been identified in break junctions, at steps of incomplete surface layers, in local confinements, and in the environment of impurities in crystals. This combined information is expected to promote understanding of electronic behaviour in such different fields as catalysis, electronic transport through gaps and interfaces and reflections at differently shaped quantum barriers.

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