



Sonderforschungsbereich 595

Elektrische Ermüdung
in Funktionswerkstoffen



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Modeling spectroscopic and structural properties of transition ions in technologically important crystals & biological systems

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Meaningful analysis of EMR and/or optical spectroscopy data for transition ions in crystals and their correlation with structural data requires advanced modeling techniques. By modeling we mean theoretical interpretation of the experimentally measurable parameters in terms of the microscopic parameters. Modeling enables also to predict the quantities measurable by EMR/optical spectroscopy and relate them to structural parameters. Illustrative examples of modeling the spectroscopic properties of iron group ($3d^N$) ions in technologically important materials and biological systems are presented. This talk provides basic understanding of physics underlying the modeling packages worked out in our group and their general capabilities.