SFB/TRR 21 - Seminar
24. November 2011, Stuttgart


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## Vibrations of quasi-free water molecules in nano-cavities of Beryl crystal lattice


Crystalline beryl ($Be_2Al_3Si_6O_{18}$:$H_2O$) offers a “simple system“ to study dynamics of separate molecules encapsulated in nano-sized cavities. In the beryl crystal, the six-membered ($SiO_4$ tetrahedra) rings stack one over another along the c-axis forming the bottle necks of 2.8 Å and cavities with diameter of 5.1 Å. In the bottle necks alkali ions (such as Na) can be located to which the $H_2O$ molecules are trapped – so called water type II. Water type I is sitting in nano-cavities and is more free. Earlier, we have performed terahertz-infrared measurements of beryl crystals and found a number of absorption lines connected with the presence of quasi-free $H_2O$ molecules of both types. In this talk we discuss mechanisms responsible for the observed water-related resonance absorptions. We associate them with optically-active transitions between energy levels of $H_2O$ molecule in parabolic potential formed by its hydrogen bonding to the cavity “walls”. In case of water-I molecules, the levels are tunnel-split due to six-fold symmetry of the potential, and we observe a rich set of transitions between the levels in different bands, governed by corresponding selection rules. Temperature dependences of absorptions will also be discussed.


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