



Seminarankündigung

**Dienstag, 3. November 2015
13:15 Uhr**

ZNN, Seminarraum EG 0.001

“Asymmetric composition dependence of lattice dynamics in $\text{MoS}_{2x}\text{Se}_{2(1-x)}$ layers ”

The mixed layered crystals allow continuous tunability of the optical band gap, rendering 2D transition metal dichalcogenide alloys appealing materials for electronic and optoelectronic device applications. Hence, characterization of these systems including understanding of the arrangement of substituting atoms in one or more layers has become fundamentally important.

In my talk, I will present the comparative Raman scattering studies of monolayer and bulk $\text{MoS}_{2x}\text{Se}_{2(1-x)}$. Contrasting reconstruction of the phonon spectrum upon dilution of one chalcogenide by the other ($x=0+$ vs $1-$) as well as apparently discontinuous features around $x=0.5$ (MoSSe) are found.

The results for bulk $\text{MoS}_{2x}\text{Se}_{2(1-x)}$ reveal two distinct sets of features related to the E_{12g} and A_{1g} modes of pure members of series. As composition x changes, the in-plane E_{12g} mode shows a two-mode behavior, whereas the out-of-plane A_{1g} mode presents more complex evolution. When x slightly increases, the four Raman peaks are identified in the range $200\text{-}280\text{ cm}^{-1}$. They evolve in different manner as composition changes, and they are divided into two types related to different distribution of the chalcogenide atoms within the $\text{MoS}_{2x}\text{Se}_{2(1-x)}$. The first type corresponds to the Se-Se case and originates at the frequency of MoSe_2 -like A_{1g} mode. The second type at higher frequencies with regard to A_{1g} mode is related to the Se-S case. Among these, at least three components are identified, shifting to higher frequency upon increasing x . They are well resolved for $0.1 < x < 0.2$, when the $2\text{Se}_2 + 1\text{SeS}$, $2\text{Se}_2 + 1\text{S}_2$ or $2\text{Se}_2 + 2\text{SeS}$ arrangements are the most probable. The frequencies of the two modes attributed to the Se-S case are not significantly affected by reducing thickness down to a monolayer, suggesting that they are related to intralayer (rather than interlayer) interaction.

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