

**S1-2.13****Excitonic Luminescence, X-ray Analysis and Local Band Structure of Chlorine Intercalated 2H- and 3R-MoS₂ polytypes**

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Photoluminescence and X-ray diffraction are used to investigate 2H and 3R polytypes of MoS₂ layered crystals intercalated with Cl₂ molecules. The spectral structure of the observed bound excitons emission is individual for each polytype, that can be used for unambiguous identification of the 2H and 3R polytypes. The DFT band structure calculations have been done for three molecular layers of 2H-MoS₂ and 3R-MoS₂ polytypes without and with intercalation of Cl₂ molecules. The spectroscopic experimental results confirmed theoretical calculations performed for both cases and it has been demonstrated that halogen intercalation completely changes the local band structure of 2H- and 3R-MoS₂ polytypes.