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Optical properties and band structure of atomically thin MoS2

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Atomically thin layers of materials can be expected to exhibit distinct electronic structure and novel properties compared to their bulk counterparts. Layered compounds, for which stable atomically thin samples can be produced, are ideal candidates for such studies. Graphene, a monolayer slice of the graphite crystal, is an illustrative example of both the stability and of the interest and importance of such materials. Here we report a study of thin layers of MoS_2, a hexagonal layered bulk semiconductor with an indirect band gap of 1.3 eV. MoS_2 samples with layer thickness N down to a monolayer were obtained by mechanical exfoliation. We observed an enhancement of the luminescence quantum yield by more than a factor of 100 in monolayer MoS_2 compared to the bulk material. The combination of absorption, photoluminescence, and photoconductivity measurements indicates that a transition to a direct-gap material occurs in the limit of the single MoS_2 layer. This result is supported by an earlier first-principles calculation [J. Phys. Chem. C **2007**, 111, 16192]. Further, by varying the thickness of the samples, we were able to probe the evolution of the electronic structure for N = 1 – 6 layers.

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