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Phase transition in MoS_2 monolayers through alloying[1]
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— Alloying of 2D monolayers can produce materials with different properties than either component. MoS_2 is known to have a stable hexagonal 1H structure, but the alternative tetragonal DT structure has been stabilized in multilayer form by Li intercalation. It is also known that the stable structure of monolayer ReS_2 is DT. In this work, we use electron microscopy and density functional theory calculations to demonstrate that an H-to-T phase transition can be achieved in MoS_2 by Re doping. Both the microscopy images and the calculations find that the phase transition occurs at a Re concentration of just below 50%. In contrast to the phase transition by lithium intercalation which is induced by the electron doping effect, the calculations find that electron doping alone, compensated by a uniform positive background, shift the critical concentration to 75%, which indicates that changes in chemical bonding facilitate the transition. At 50% alloying, the energy gap of the DT material is only 0.2 eV, compared with 1.8 eV in 1H MoS_2.

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