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**Efficient n-type doping of $MoO_3$**[1] HARTWIN PEELAERS, CHRIS G. VAN DE WALLE, University of California, Santa Barbara — $MoO_3$ is a layered material that has shown great promise as a transparent contact to organic photovoltaics and organic light-emitting diodes. It also exhibits photo- and electrochromic properties, and can be used as catalyst or sensor material. Due to its capability to reversibly accommodate Li it can be used in Li batteries. Despite these interesting properties, remarkably little is known about the properties of native defects and the possibilities of controlling the properties by intentional doping. We have used advanced hybrid functional calculations within density functional theory to investigate efficient doping strategies for this material. In particular, we explored the role of native defects in the conductivity of this material. To control the n-type conductivity and to obtain a larger amount of free carriers, intentional dopants can be used. We show that substitutional Re (on a Mo site) is a shallow donor. In contrast, substitutional doping with Mn, which also has one additional electron compared to Mo, leads to compensating behavior. Halogen impurities on the O site also act as shallow donors.

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