Metalization of Li$_2$S Nanoparticles in Li-S batteries

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FIG. 1: Atomic structures of (c,d) unreconstructed stoichiometric and (a,b,e,f) non-stoichiometric Li$_2$S(111) surfaces that have been considered to plot the Figure 4 of the manuscript.

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FIG. 2: Atomic structures of the (a,c) reconstructed and (b) unreconstructed stoichiometric as well as (d–g) non-stoichiometric Li$_2$S(100) surfaces that have been considered to plot the Figure 4 of the manuscript.
FIG. 3: Atomic structures of (a) unreconstructed stoichiometric and (b–e) non-stoichiometric Li$_2$S(110) surfaces that have been considered to plot the Figure 4 of the manuscript.