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Jahn-Teller distortion and magnetic ordering in layered nickelates MICHELLE JOHANNES, IGOR MAZIN, NOAM BERNSTEIN, Naval Research Laboratory — One of the long-standing challenges in the theory of layered nickelates is that $NaNiO_2$ is antiferromagnetic and has a strong Jahn-Teller induced orbital ordering, while $LiNiO_2$ has none. A variety of hypothesis have been proposed to explain this mystery: a difference in Li/Na ionic radii, differences in the underlying electronic structure, the zero-point motion of Li ions, etc. One of the most viable propositions is that the difference is due to the presence of $Na2^+$ ions (1% or more) on the Li sites. It remains unclear whether the magnetic interaction of $Na2^+$ with the in-plane $Na3^+$ is strong enough to cancel the Li-assisted antiferromagnetic superexchange even for 1% of $Na2^+$, and what effect it has on orbital ordering. We provide quantitative arguments, based on first principles calculations and atomistic simulations, that spin and orbital orderings are unrelated, and that both are destroyed (the latter in a rather unusual way) by $Na2^+$ impurities, but for entirely separate reasons.

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