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Abstract for an Invited Paper
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Designing Magnetism in Oxide Superlattices¹

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Dramatic improvements in pulsed laser deposition and oxide molecular beam epitaxy suggest that it may be possible to create “designer” materials with desired correlated electron properties. This talk presents the results of theoretical studies based on the density functional plus dynamical mean field approximation aimed at determining design rules for creating or optimizing magnetism in oxide superlattices. Among the topics covered will be the physics of long-period antiferromagnetic states in nickelate-based heterostructures and the relation of strain-induced octahedral rotations in creating ferromagnetic states in vanadate-based superlattices. We show in particular how appropriately designed superlattices may lead to structure-doping combinations which do not occur in bulk solid solutions but which can produce high Curie temperature ferromagnetism. Limitations of present theoretical capabilities and opportunities and needs for conceptual, methodological and algorithmic improvements will also be discussed. This work is based in part on collaborations with C. Marianetti, B. Lao and H-T Dang.

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