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Abstract for an Invited Paper
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Predicting and Controlling the Electronic, Spin and Lattice Degrees of Freedom of Artificial Atoms in Solids[1]

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Recent work has focused on identifying new defect qubits in 3D and 2D materials with quantum optoelectronic properties that reach beyond the limitations of the well-known nitrogen-vacancy (NV-) center in diamond. Group IV-vacancy centers in diamond have been of particular interest due to their symmetry-protected optical transitions and long-lived spin degree of freedom. In the first part of my talk I will discuss the ground- and excited-state properties of group IV centers in their negative and neutral charge state with a focus on the dynamic and product Jahn-Teller (pJT) effects, including their impact on zero phonon line energetics, spin-orbit coupling and lattice dynamics. From first principles, I will show how we capture the interplay of spin-orbit and electron-phonon coupling in order to accurately describe the pJT-affected excited state manifold, going beyond a perturbative description. In the second part of my talk I will present our recent work on color centers in low dimensional materials in particular the impact of localized strain and strong-spin orbit coupling. I will conclude with discussing schemes for selective control of optically active qubits of differing excitation energies towards creating components for quantum networks.

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