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**Accurate donor electron wave functions from a multivalley effective mass theory.**[1] LUKE PENDO, XUEDONG HU, SUNY – University at Buffalo — Multivalley effective mass (MEM) theories combine physical intuition with a marginal need for computational resources, but they tend to be insensitive to variations in the wavefunction. However, recent papers suggest full Bloch functions and suitable central cell donor potential corrections are essential to replicating qualitative and quantitative features of the wavefunction [1,2]. In this talk, we consider a variational MEM method that can accurately predict both spectrum and wavefunction of isolated phosphorus donors. As per Gamble et. al [1], we employ a truncated series representation of the Bloch function with a tetrahedrally symmetric central cell correction. We use a dynamic dielectric constant, a feature commonly seen in tight-binding methods. Uniquely, we use a freely extensible basis of either all Slater- or all Gaussian-type functions. With a large basis able to capture the influence of higher energy eigenstates, this method is well positioned to consider the influence of external perturbations, such as electric field or applied strain, on the charge density. [1] JK Gamble, et al., Phys. Rev. B **91**, 235318 (2015) [2] AL Saraiva, et al., Phys. Rev. B **93**, 045303 (2016)

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