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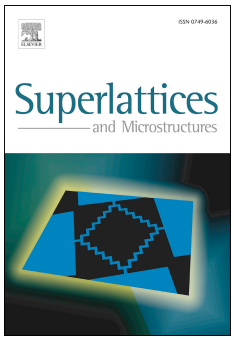

A two-band spinful k.p Hamiltonian of monolayer MoS_2 from a nine-band model based on group theory

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Graphical Abstract

$$H_0 = \frac{p^2}{2m} + V(r)$$

$$H_{fe} = \frac{\hbar^2 q^2}{2m_e}\mathbb{1}_9$$

$$H_{\mathbf{k}.\mathbf{p}} = \frac{\hbar \mathbf{q}.\mathbf{p}}{m_e}$$

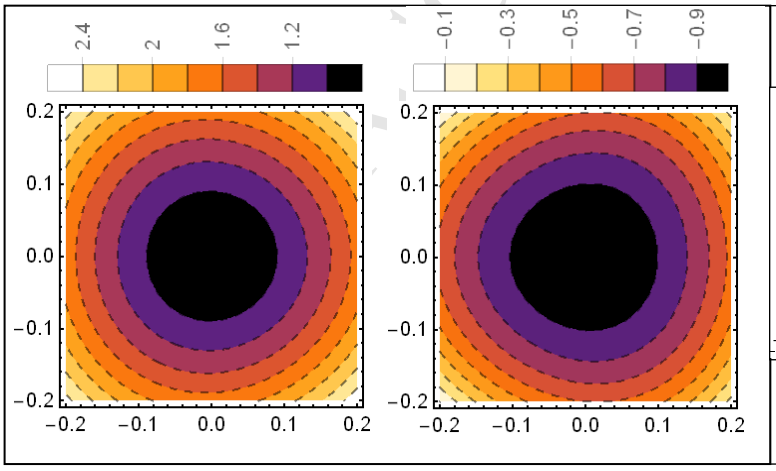
$$H_{SO} = \frac{\hbar}{4m_e^2 c^2}\frac{1}{r}\frac{dV(r)}{dr}\hat{\mathbf{L}}.\hat{\mathbf{S}}$$

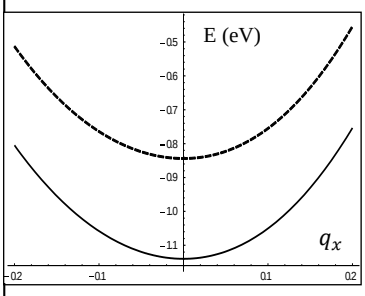
$$H = H_0 + H_{fe} + H_{k.p} + H_{SO}$$

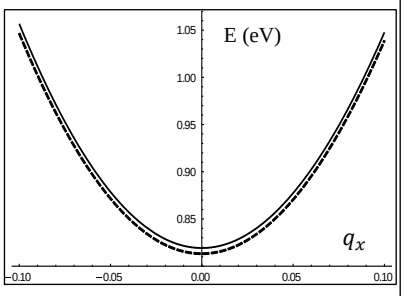
$$\left\{\left|\Psi_{E_1'}^{vb-5},s\right\rangle,\left|\Psi_{A'}^{vb-4},s\right\rangle,\left|\Psi_{E_2'}^{vb-3},s\right\rangle,\left|\Psi_{E_1''}^{vb-2},s\right\rangle,\left|\Psi_{E_2''}^{vb-1},s\right\rangle,\left|\Psi_{A'}^{vb},s\right\rangle,\left|\Psi_{E_1'}^{cb},s\right\rangle,\left|\Psi_{A''}^{cb+1},s\right\rangle,\left|\Psi_{E_2'}^{cb+2},\right.\right.$$

By using Löwdin partitioning method

$$H_{eff}^{\tau,s} = \begin{bmatrix} \varepsilon_{cb} + \frac{\hbar^2}{2m_e}q^2 + \alpha_{\tau,s}q^2 + \lambda_1^{\tau,s}\tau|q|^3\cos(3\varphi) + \tau\Delta_c s_z & \tau\gamma_3^* q_+ + \kappa_{\tau,s}q_-^2 + \lambda_3^{\tau,s}\tau q_+|q|^2 \\ \tau\gamma_3 q_- + \kappa_{\tau,s}^* q_+^2 + \lambda_3^{\tau,s}\tau q_-|q|^2 & \varepsilon_{vb} + \frac{\hbar^2}{2m_e}q^2 + \beta_{\tau,s}q^2 + \lambda_2^{\tau,s}\tau|q|^3\cos(3\varphi) + \tau\Delta_v s_z \end{bmatrix}$$







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