In This Lecture:

- Two-dimensional Materials:
  Transition Metal Dichalcogenides
Periodic Table

TMDs

Periodic Table with annotations and highlights.
Orbital Profiles: \( R_{nl}(r) \ Y_{lm}(\theta, \phi) \)

Radial Dependence: \( R_{nl}(r) \)
- det'd by \( r \)
- \( \exp(-qr) \) as \( r \to \infty \)

Polar Dependence: \( P_{l}^{m}(\cos \theta) \)

Azimuthal Dependence: \( \sin m \phi, \cos m \phi \)

Latitudes: \( l-1m \) nodal lines
- \( l \) nodal lines
- \( |m| \) nodal lines
C. Bulutay  
Topics on Semiconductor Physics  

\[ S \ (l=0) \]

\[ P \ (l=1) \]

\[ d \ (l=2) \]

\[ f \ (l=3) \]

\[ m=0 \]

\[ m=\pm 1 \]

\[ m=\pm 2 \]

\[ E - d_{x^2-y^2} \]

\[ E - d_{x y} \]

\[ E - d_{x^2} \]

\[ E - d_{z^2} \]

"2" of these

"2" of these

"2" of these

"2" of these
**d-orbital electronics**

New in se/c’s

orbitals lie in the x-y, x-z, and the y-z planes (but not along any of the axes)

Mo: [Kr]. $5d^5.6s^1$
W: [Xe].$4f^{14}.5d^4.6s^2$

Source: socratic.org
Graphene versus TMDs

Graphene $\rightarrow$ single sheet

Source: cnx.org

TMD MX$_2$ $\rightarrow$ multilayer/monolayer

Source: Yazyev Materials Today 2015
TMDs: bulk vs monolayer

Source: Yazyev Materials Today 2015
TMDs: atomic orbitals

![Graphs showing energy bands and atomic orbital weights](image)

Figure 3. Atomic orbital weights in the energy bands of MX$_2$. (a) $d$ orbitals of the metal atom, and (b) $p$ orbitals of the chalcogen atoms. The size of each symbol is proportional to the weight of the atomic orbital. SOC was neglected in these calculations.

**Source:** Kormanyos et al. 2D Matl. 2015
Figure 2. Overview of the band structure of monolayer TMDCs as obtained from DFT calculations. (a) Dispersion along the $\Gamma$–K–M–$\Gamma$ line in the BZ. SOC is taken into account. Various band-edge energy differences and spin-splittings are also indicated; for definitions see the main text. (b) Dispersion of the VB as a function of the wavevector $k$ in the whole BZ. The hexagonal BZ is denoted by thick black lines. (c) The same as (b) for the CB. In (b) and (c) SOC is neglected.

Source: Kormanyos et al. 2D Matl. 2015
Valley Optical Selections

Valleytronics with Alloying

A & B Excitons under Zeeman Effect

k.p for TMDs: for $K^\pm$ valleys

\[ \mathcal{H}_E^\pm(q) = \mathcal{H}_1^\pm(q) + \mathcal{H}_2^\pm(q), \]

\[ \mathcal{H}_1^\pm(q) = \begin{pmatrix}
E_{v-5} & \delta_7 q_- & \delta_6 q_+ & \delta_4 q_- & 0 & \delta_2 q_+ \\
\delta_7 q_+ & E_{v-4} & \delta_5 q_- & 0 & \delta_3 q_+ & \delta_1 q_- \\
\delta_6 q_- & \delta_5 q_+ & E_{v-3} & \gamma_2 q_- & \gamma_5 q_- & 0 \\
\delta_4 q_+ & 0 & \gamma_3 q_- & E_{v} & \gamma_3 q_+ & \gamma_4 q_- \\
0 & \delta_3 q_- & \gamma_5 q_+ & \gamma_3 q_- & E_c & \gamma_6 q_- \\
\delta_2 q_- & \delta_1 q_+ & 0 & \gamma_4 q_+ & \gamma_6 q_- & E_{c+2}
\end{pmatrix}, \]

\[ [\mathcal{H}_2^\pm(q)]_{nl} = \frac{\hbar^2 q^2}{2m'_n} \delta_{nl}, \ n, l = 1..6 \]

\[ q_\pm = q_x \pm iq_y, \quad q^2 = q_x^2 + q_y^2 \]

Source: Rybkovksy et al. arXiv: 1610.02695
TABLE III. Parameters of the $k \cdot p$ model as introduced in Eqs. (6), (7). The values of $\gamma_i$ and $\delta_i$ are given in eVÅ, the units of $E_i$ are eV, the effective masses $m_i'$ are given in the units of $m_0$. Parameterizations are based on TB models listed in footnotes.

<table>
<thead>
<tr>
<th></th>
<th>MoS$_2$ a</th>
<th>MoS$_2$ b</th>
<th>MoS$_2$ c</th>
<th>MoS$_2$ d</th>
<th>MoS$_2$ e</th>
<th>MoSe$_2$ f</th>
<th>WS$_3$ g</th>
<th>WSe$_2$ h</th>
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<td>$E_{v-5}$</td>
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<td>2.44</td>
<td>1.52</td>
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<td>$E_{c+2}$</td>
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<td>2.98</td>
<td>4.04</td>
<td>3.96</td>
<td>4.60</td>
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<td>$\delta_5$</td>
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<td>$\delta_6$</td>
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<td>0.69</td>
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<td>$m'_{v-5}$</td>
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<tr>
<td>$m'_{v-4}$</td>
<td>1.34</td>
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<td>2.00</td>
<td>1.22</td>
<td>0.78</td>
<td>0.84</td>
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<td>$m'_{v-3}$</td>
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<td>6.92</td>
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<td>$m'_v$</td>
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<td>$m'_{c}$</td>
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<tr>
<td>$m'_{c+2}$</td>
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<td>-0.63</td>
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</tr>
</tbody>
</table>

Source: Rybkovksy et al. arXiv: 1610.02695
**k.p for TMDs**

![Graph of electronic spectra of MoS$_2$](image)

**FIG. 1.** Electronic spectra of MoS$_2$ calculated using TB models H. Rostami et al. [26] (a) and S. Fang et al. [24] (b). Red lines are $k \cdot p$ quadratic dispersions at $K$-point calculated using effective masses for each band (see text for details). Note the different order of deep valence bands in two panels.

**Source:** Rybkovksy et al. arXiv: 1610.02695