1. Background

- High power electromagnetic wave signal
- \( \Phi = r^2 \)
- It is well-known that adsorption of alkaline, or alkaline-earth metals/metal-oxide on transition metals lowers work function.

2. Computational Process

- Schrödinger Equation:
  \[
  \frac{-\hbar^2}{2m} \sum_{j=1}^{N} \nabla_j^2 \Psi(r_j) + \sum_{j<k} V(r_{jk}) + \sum_{j=1}^{N} \int [V(r_j, r_j)] \Psi = E \Psi
  \]
- Initial Guess \( n(r) \)
- Calculate Potential \( V_{\text{eff}}(r) = V(r) + \frac{e^2}{r_{\text{kin}}} + V_{\text{xc}}[n(r)] \)
- Solve Kohn-Sham (Single Electron) Equations:
  \[
  \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{eff}}(r) \right] \psi_i = \epsilon_i \psi_i
  \]
- Evaluate \( n(r) \) and \( E \)
  \[
  n(r) = \frac{1}{2m} \sum_{j} \psi_j^2 \psi_j^* \psi_j
  \]
- Output: Energy, Forces, Structures, Properties

3. Materials Discovery--Bulk

- The ground states structures of Os-W alloys
- Configurations of O/W, and possible positions for Ba tungsten (001)
- Configurations of Ba,Sc,O adsorptions on tungsten
- Stability is evaluated by surface energy
  \[
  \gamma_s = \frac{E([\text{Ba}_x \text{Sc}_y O_z W_s] - nE[\text{W}_s]) - x\mu_{\text{Ba}} + y\mu_{\text{Sc}} + z\mu_{O})}{2A}
  \]

4. Materials Discovery--Surface

- It is well-known that adsorption of alkaline, or alkaline-earth metals/metal-oxide on transition metals lowers work function.
- Configurations of O/W, and possible positions for Ba tungsten (001)
- Configurations of Ba,Sc,O adsorptions on tungsten
- Stability is evaluated by surface energy
  \[
  \gamma_s = \frac{E([\text{Ba}_x \text{Sc}_y O_z W_s] - nE[\text{W}_s]) - x\mu_{\text{Ba}} + y\mu_{\text{Sc}} + z\mu_{O})}{2A}
  \]

5. Materials Characterization

- Richardson Formula:
  \[
  J = A_0 e^{\frac{-\Phi}{kT}}
  \]

6. Materials and Device Design

- With \( \gamma_{(001)}, \gamma_{(110)}, \) and \( \gamma_{(112)} \) known, crystal shape can be calculated for every possible set of configurations.

7. Summary and Future Work

- Role of Sc: tune \( O_2 \) chemical potential
- Future work:
  - Further experiments to verify the computational work;
  - Fabricate improved cathodes by tuning

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**Legend format:** [[(001), (112), (min(\( \mu_{Ba}, \mu_{O}, \mu_{Sc} \)))]

**Ranges of \( \mu_{Ba}, \mu_{O}, \) and \( \mu_{Sc} \):**

- Stable
- Have very low \( \Phi \):
- Yield right crystal shape;