ELI-ALPS Research Institute
TOWARDS THE SHARP END OF ATTOSCIENCE

'EUCALL Joint Foresight Topical Workshop:
Theory and Simulation of Photon-Matter Interaction'

Superior Photo-thermionic electron Emission from Illuminated Phosphorene Surface

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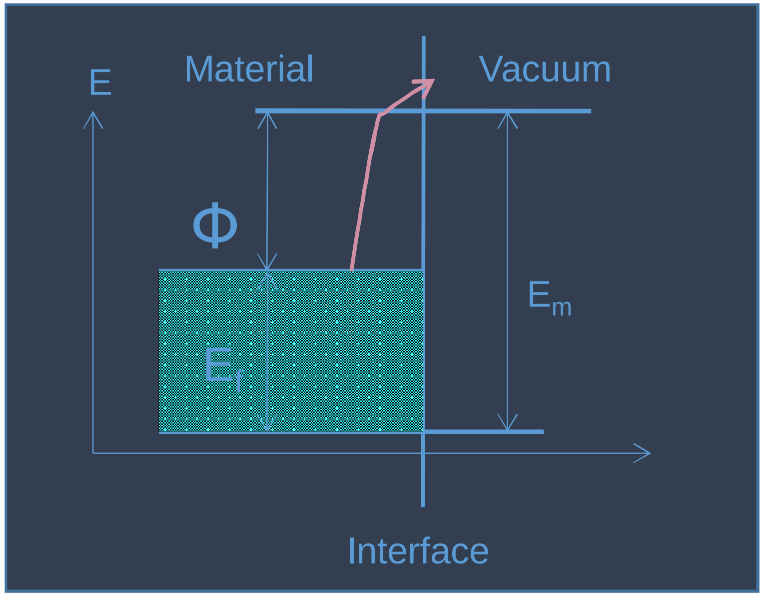
Electron emission



- Completely filled valence band-till Fermi level
- Pulled back due to electromagnetic forces
- Requires sufficient energy to overcome these forces
- Φ = work function (material specific). The energy required for an electron to escape in to the vacuum.

$J_c = A_c T^2 \exp(-\Phi/kT)$ in A/cm^2
A_c = material dependent constant
T = emission temperature
k = Botzmann's constant
As barrier height Φ reduces, J_c increases

Material properties, dimensionality, suitable energy-dispersion relation, workfunction, etc play major role in electron emission

Different electron emission processes

1

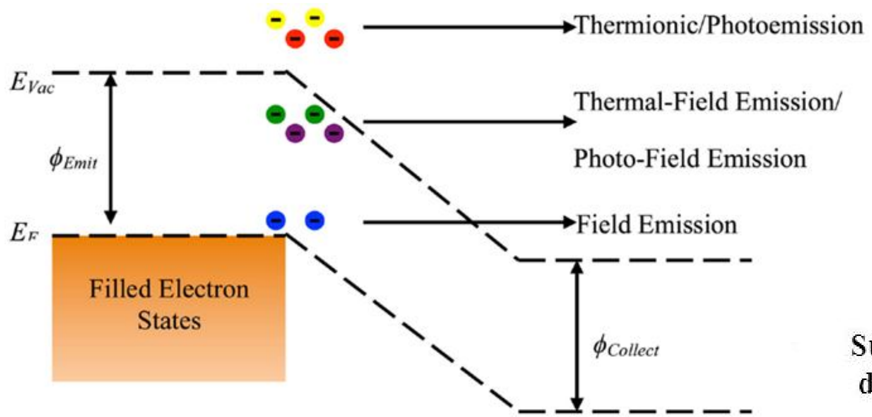
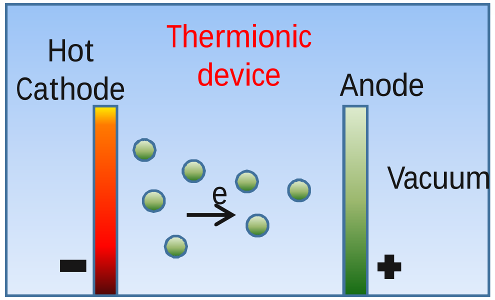
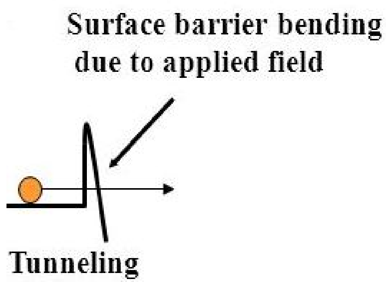


Fig: Energy Diagram





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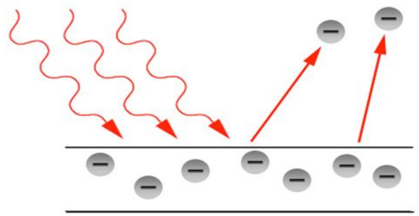
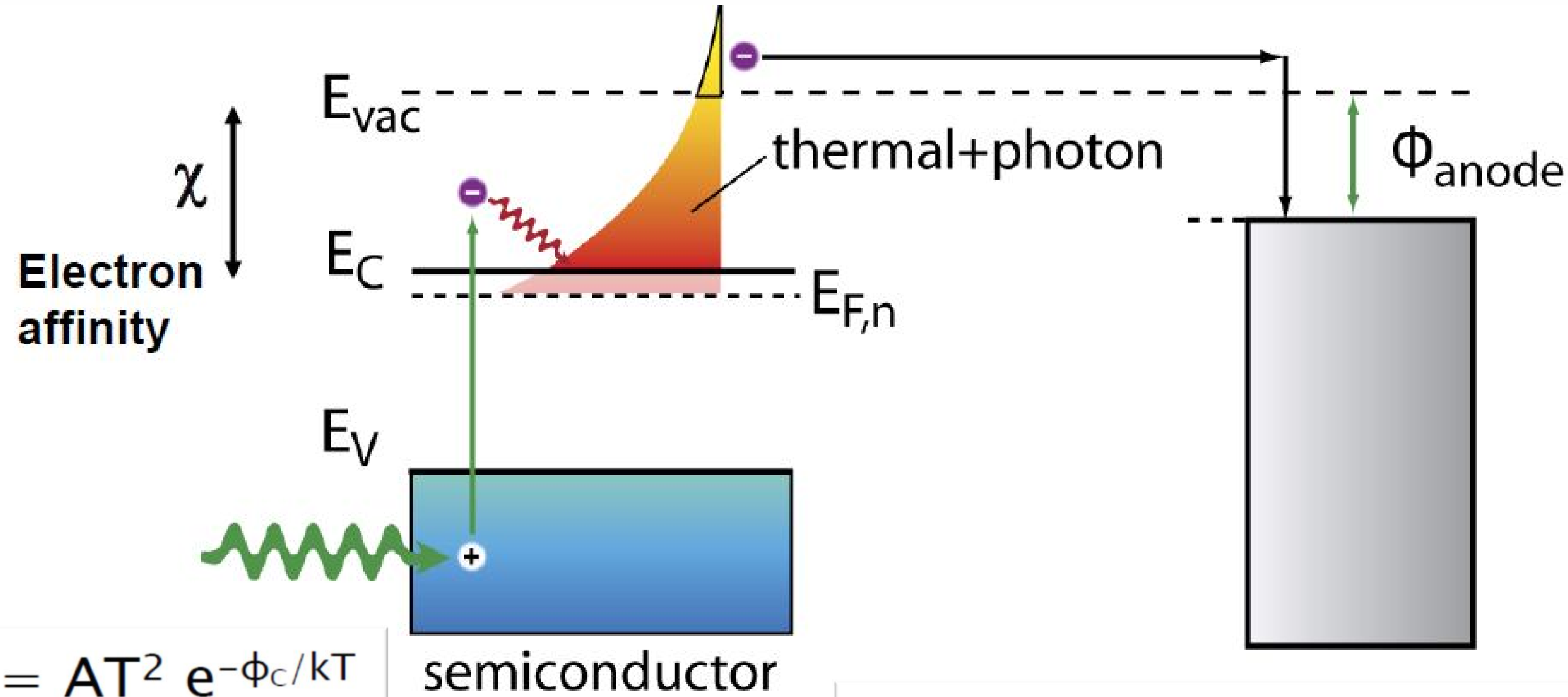


- Electron gains energy from external sources light heat or light and results in thermionic or photoelectric emission, respectively
- Decrease in barrier height when field is applied – electrons tunnel through the barrier: Field emission

Barrier height and electron emission are effected by external excitation

[1] Patrick et al, Front. Energy Res., 2014
[2] https://www.thoughtco.com/the-photoelectric-effect-2699352

Combine photon absorption with thermionic emission?

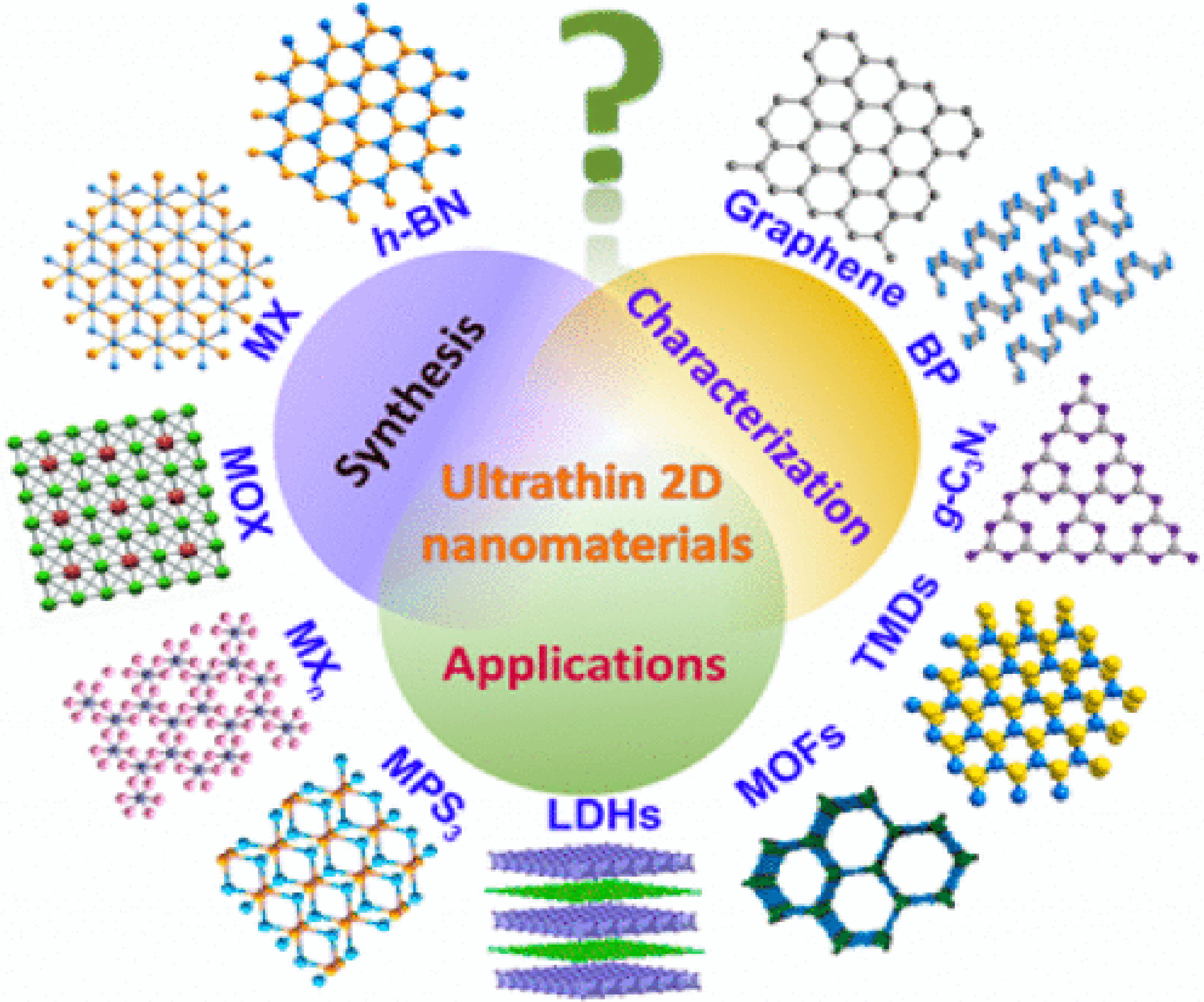


$$J = AT^2 e^{-\phi_C/kT}$$
$$P = J(\phi_C - \phi_A)$$

$$J = AT^2 e^{-\phi_C/kT} e^{\Delta E_f/kT}$$

- Photo-excited carriers into conduction band
- Thermionically emit these excited carriers
- Electrons have to overcome electron affinity barrier (not full work-function)
- Finally collected at low work-function anode

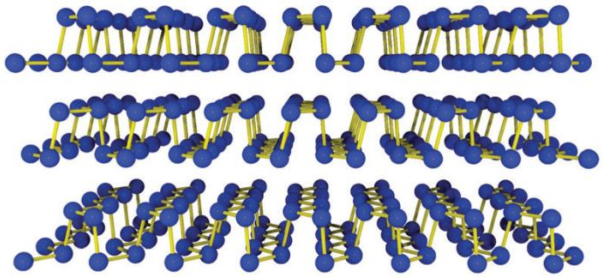
Wide range of 2D materials



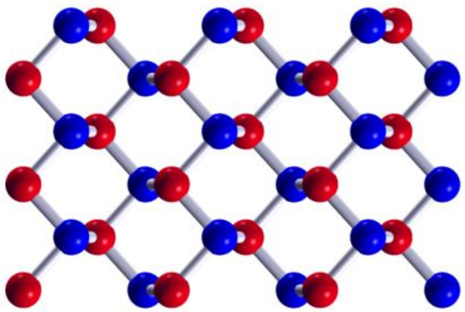
- 2D systems, with range of electronic structures.
- Different electron dynamics manifest in them.
- Formation of multiple hybrid 2D systems possible.

Overview of 2D Phosphorene

1 **Black-Phosphorous**



2D Black-Phosphorene

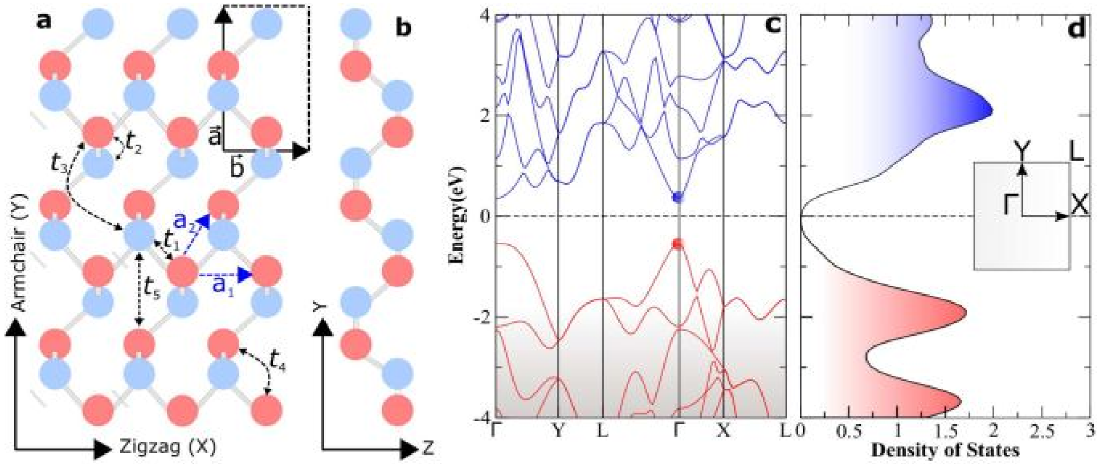


- Most stable allotrope
- Layered structure
- vdW interactions between layers
- Synthesized in 1914 by Bridgman

- Covalent bonding between atoms in a layer - to form a puckered honeycomb structure - nonplanar.
- Anisotropic structure {unlike graphene}

[1] Wang et al., Journal of applied physics 117, 124302 (2015)

Phosphorene & its band structure and density of states



- Direct band gap of ~1eV
- Fermi level is set to zero

- Tuning of <u>Tight-Binding</u> parameters to reproduce <u>DFT</u> results of energy bands near fermi level

Effective tight-binding (TB) Hamiltonian for phosphorene[1]:

$$H = \sum_{(i,j)} t_{ij} c_i^{\dagger} c_j$$

i.e. $H = \sum_{\mathbf{k}} c^{\dagger}(\mathbf{k})\, \hat{H}'_{\mathbf{k}}\, c(\mathbf{k})$, where $\hat{H}'_{\mathbf{k}} = \begin{pmatrix} T^4(\mathbf{k}) & T^0(\mathbf{k}) \\ T^{0*}(\mathbf{k}) & T^4(\mathbf{k}) \end{pmatrix}$,

Usual parabolic dispersion energy relation is no longer valid for reduced dimensional materials. DFT / TB model based is suitable for E-k relation.

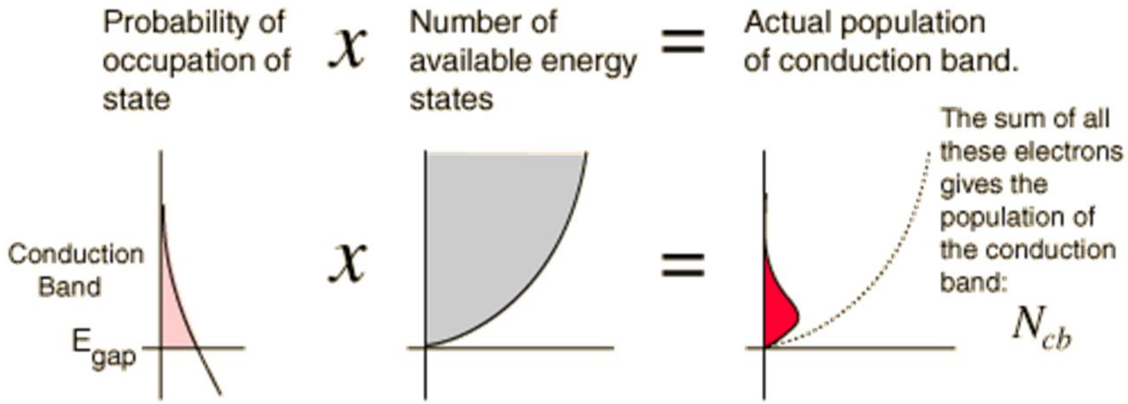
[1]. A.N. Rudenko et al., Phys. Rev. B **89**, 201408(R)

Fermi energy and Carrier concentration

- Density of electronic states is given by density of available energy states times the probability of occupation
- Density of electrons in an interval E and E+ΔE=
  density of states x probability of occupancy x energy interval

$$dN = D(E) \cdot F(E,T) \cdot dE$$

- Probability of occupancy: Fermi-Dirac distribution $F(E,T)=\frac{1}{e^{\frac{E-E_F}{kT}}+1}$



- Concentration of electrons ready to emit = $\int D(E).\ F(E,T)dE$

Results: Dependence of emission current on workfunction

- Photo-thermionic current dominates over thermionic current at low temperature
- Significant flux at lower temperatures promotes design of photon irradiated phosphorene for photothermionic convertors
- Anisotropic phosphorene shows higher emission current than graphene (linear parallel dispersion), which is utilised as efficient thermionic conversion
- Anisotropy feature may be exploited in fabricated phosphorene based cathodes in thermionic conversion schemes

Results: comparison with experimental values

Current Vs tuned barrier height

- Experimental work[1] on electronic transport characteristics of field effect transistors
- However, their result also unravels the thermionic emission aspect relevant to our study
- Shaded region corresponds to experimental conditions
- Agrees well with experimental data

[1]. S. Das et al., Nano Lett., **2014**, 14 (10)

Summary and outlook

- We demonstrate that 2D phosphorene has the potential to be a good photo-thermionic electron emitter
- Semi-analytical modelling to calculate thermionic emission flux and prescribed how this flux can be enhanced by photon irradiation
- Anisotropic energy dispersion of phosphorene results in higher emission flux when compared to those from graphene
- This approach helps in understanding photo-thermionic behaviour of phosphorene with features that matches well with experimental results
- Next aim is to incorporate higher order complexity in our approach that deals with non-adiabatic spatio-temporal dependent aspects

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THANK YOU
FOR YOUR
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