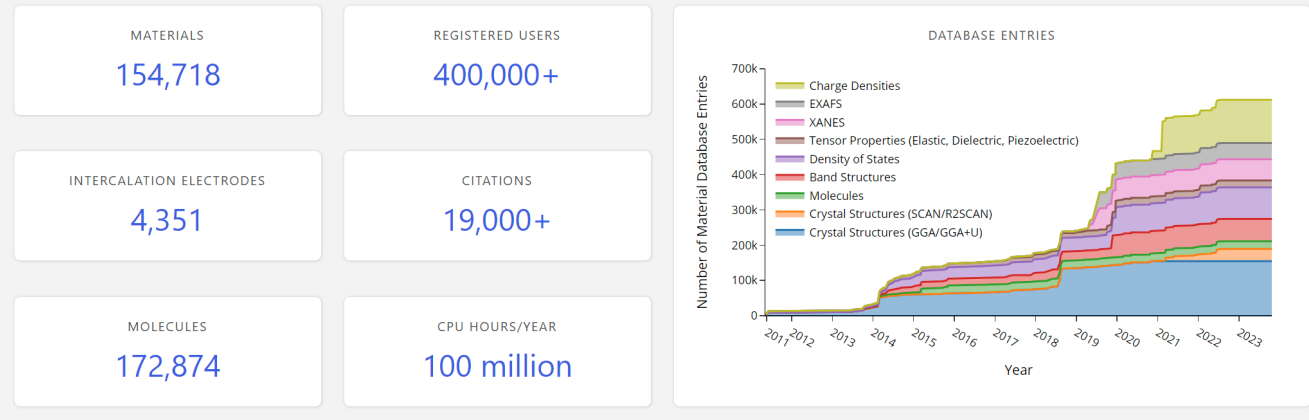


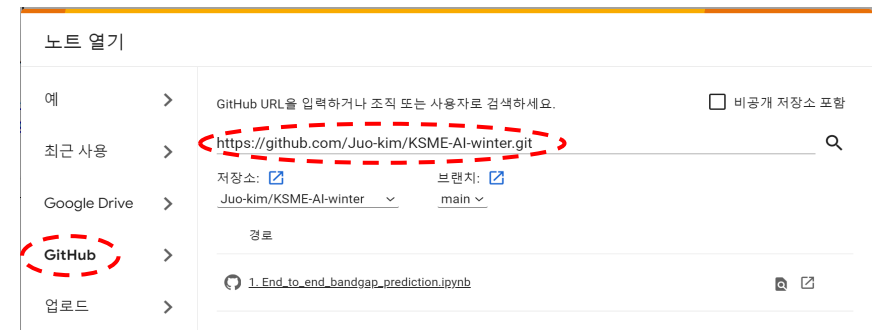
실습 자료 안내

The Materials Project by the numbers



- 15만여개 Inorganic 물질에 대한 DFT 계산 정보를 포함하고 있는 Materials Project 데이터 베이스 활용
- 물질의 전자 상태를 나타내는 값인 Bandgap 예측하는 모델 생성

- Colab 접속 (<https://colab.google/>)
- 파일 → 노트 열기 → GitHub → URL 검색



URL : <https://github.com/Juo-kim/KSME-AI-winter.git>

KSME-AI-winter

Juo Kim

CS-AI Lab

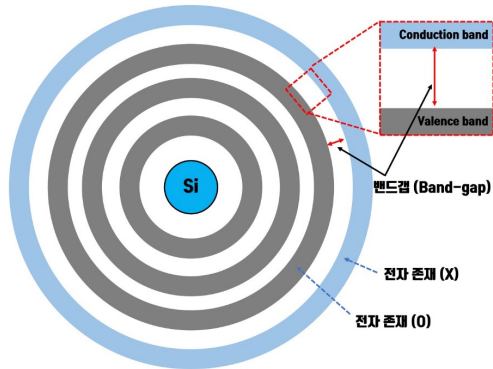
School of Mechanical Engineering
Soongsil University

Contact : rlawndh14@gmail.com

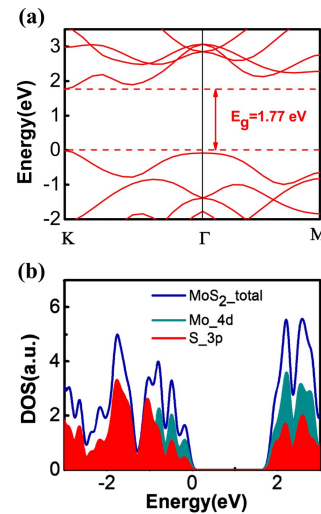


Bandgap?

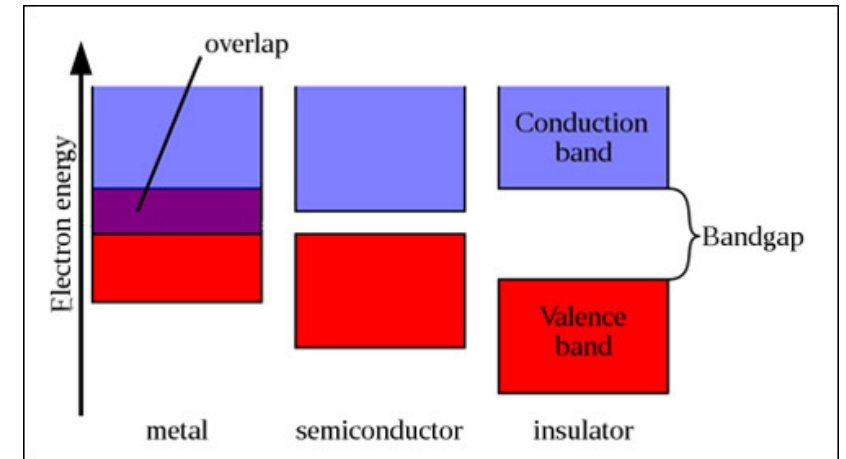
- Energy gap : 전자가 존재하고 있는 가장 높은 에너지 레벨 (Valence Band) 부터 전자가 존재하지 않는 가장 낮은 에너지레벨 (Conduction Band) 사이의 에너지 준위
- 물질이 외부에서 충분한 에너지를 공급받게 된다면, Valence band에 위치한 전자가 Conduction Band로 뛰어넘는 것이 가능함
- Bandgap의 크기에 따라 물질의 전기적 성질을 확인할 수 있음
- Metal = 0 eV, 0 eV < Semiconductor < 4 eV, Insulator \geq 4 eV
- 전기적 성질을 알아보기 위해서 매우 중요하지만, Bandgap 계산을 위해 필요한 계산적, 실험적 cost가 큼



<https://j-science.tistory.com/11>



DOI: [10.1186/1556-276X-9-676](https://doi.org/10.1186/1556-276X-9-676)



http://solarcellcentral.com/junction_page.html

Materials Project

- Open source Inorganic database 중 하나
- 154,718개의 Inorganic 물질에 대한 DFT 계산 기반의 물성 포함
- Bandgap, Energy above hull, Space group number, Crystal structure 등 많은 계산 결과

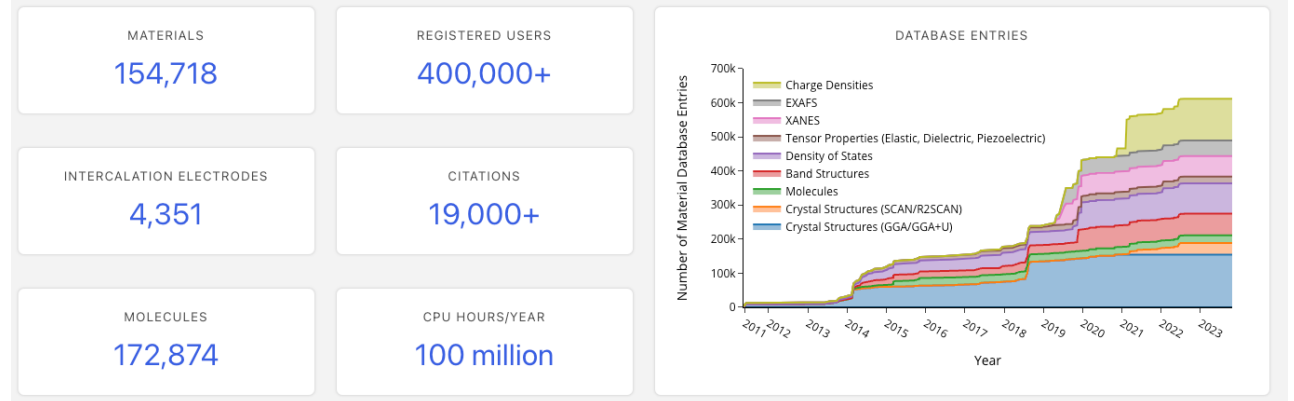
→ Materials Project database로 bandgap을 예측할 수 있는 regression model을 만드는 것이 실습의 목표



The Materials Project

Harnessing the power of supercomputing and state-of-the-art methods, the Materials Project provides open web-based access to computed information on known and predicted materials as well as powerful analysis tools to inspire and design novel materials.

The Materials Project by the numbers



PHYSICAL REVIEW B

covering condensed matter and materials physics

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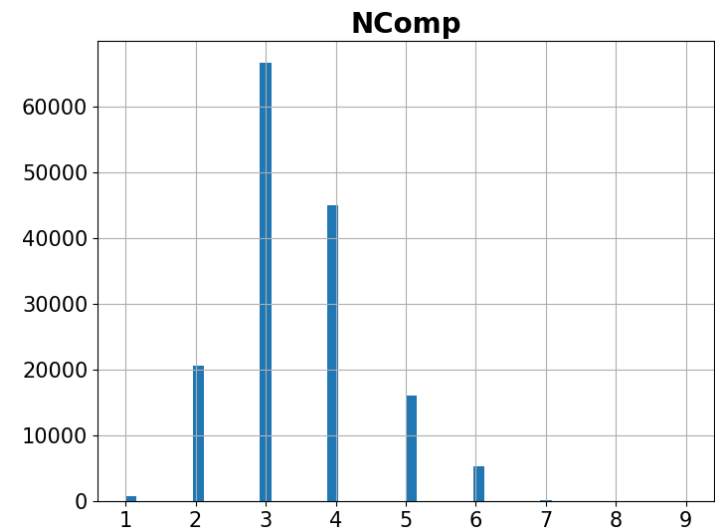
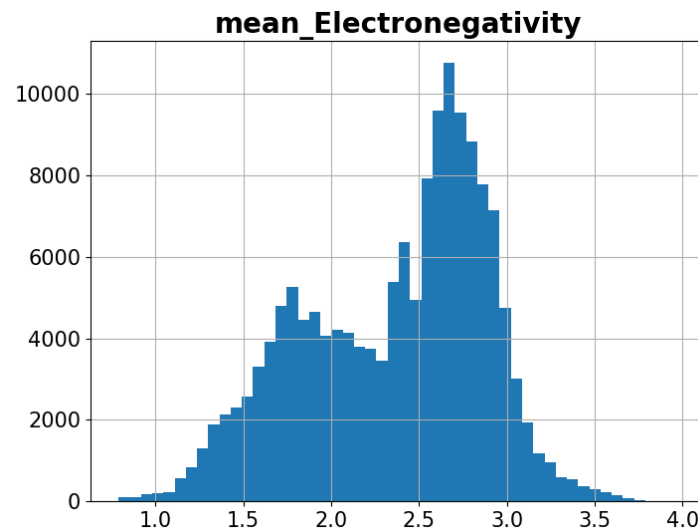
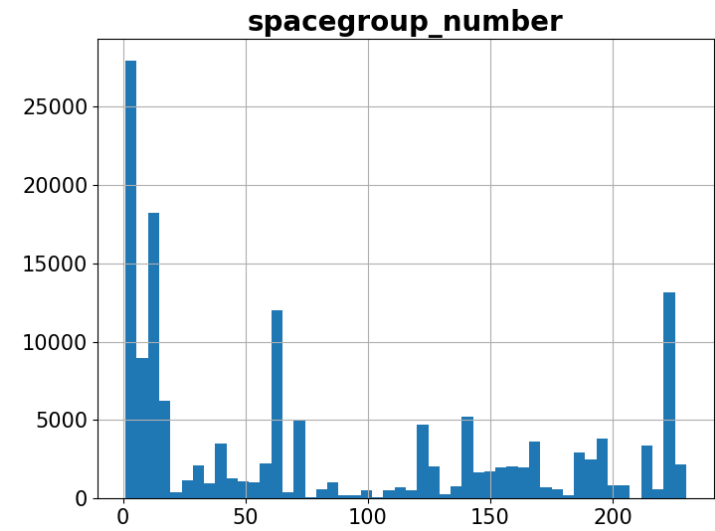
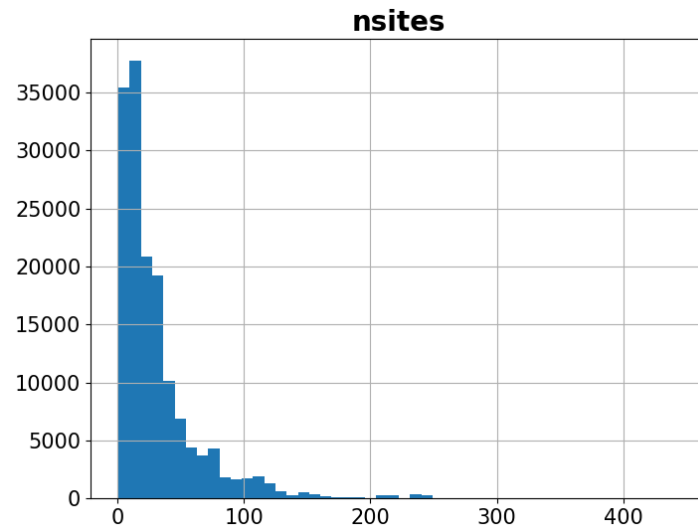
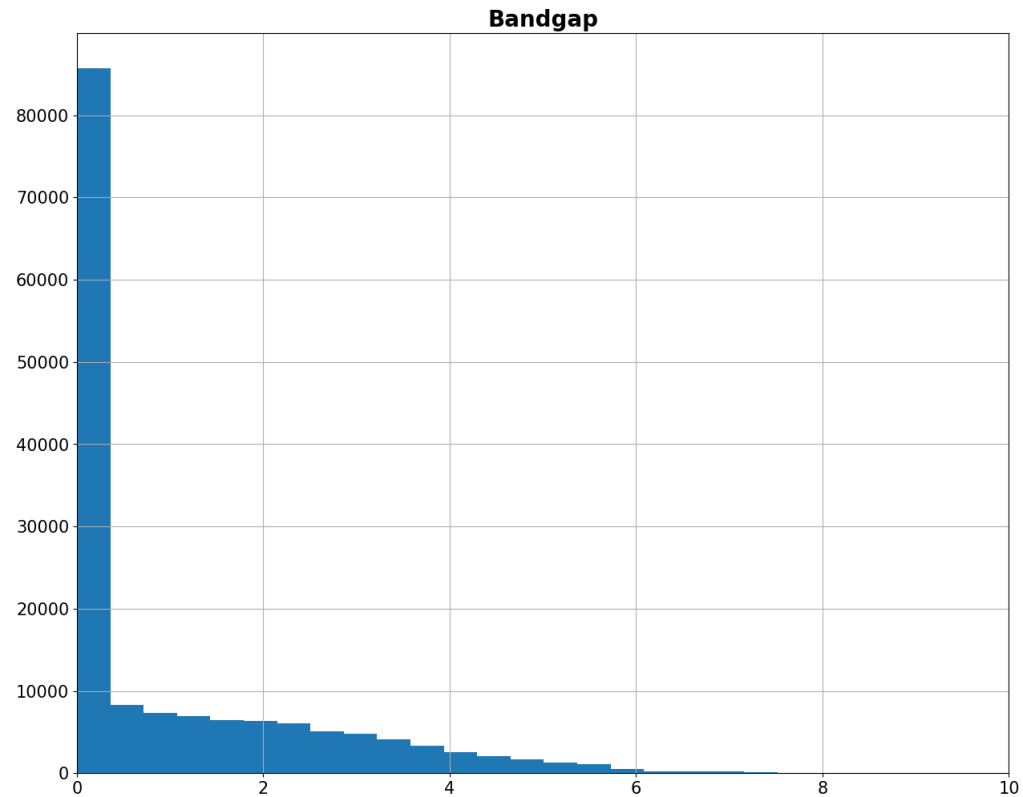
Including crystal structure attributes in machine learning models of formation energies via Voronoi tessellations

Logan Ward, Ruoqian Liu, Amar Krishna, Vinay I. Hegde, Ankit Agrawal, Alok Choudhary, and Chris Wolverton
Phys. Rev. B **96**, 024104 – Published 14 July 2017

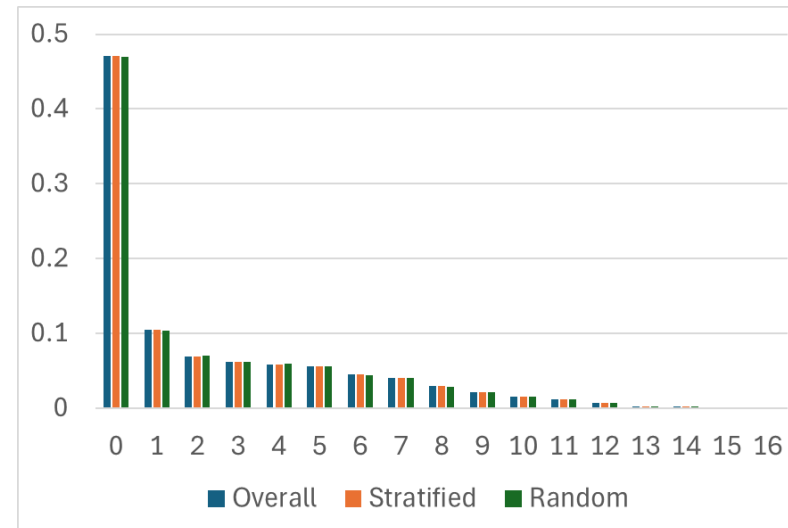
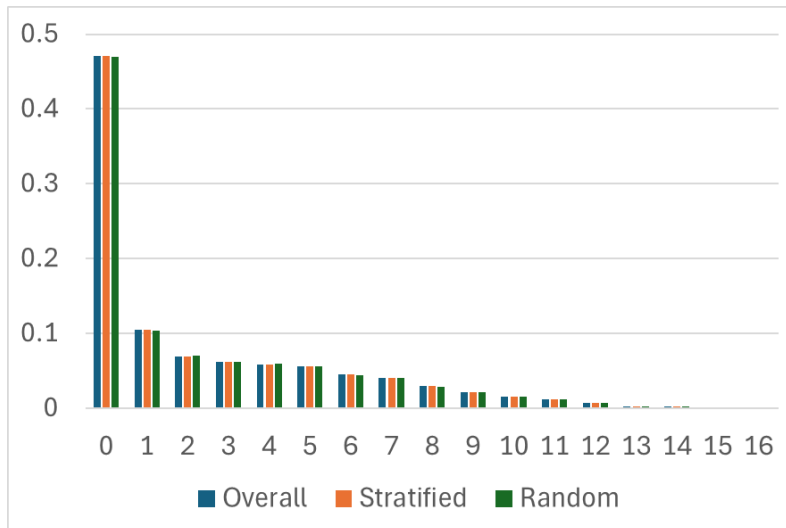
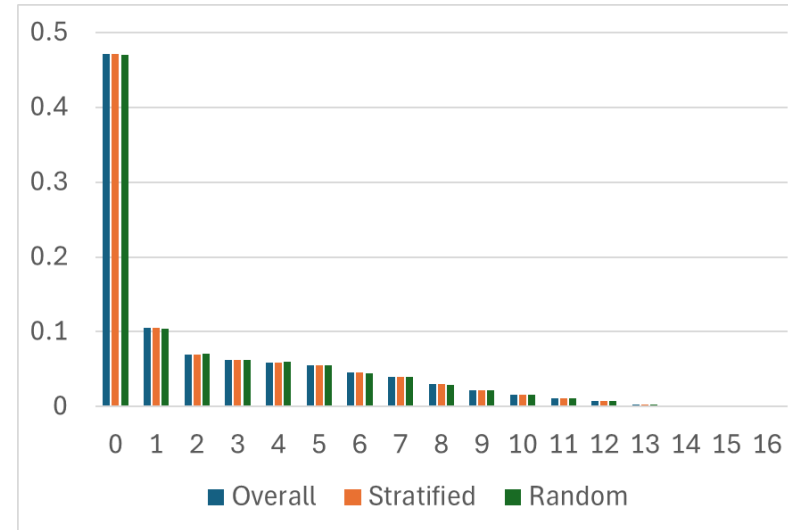
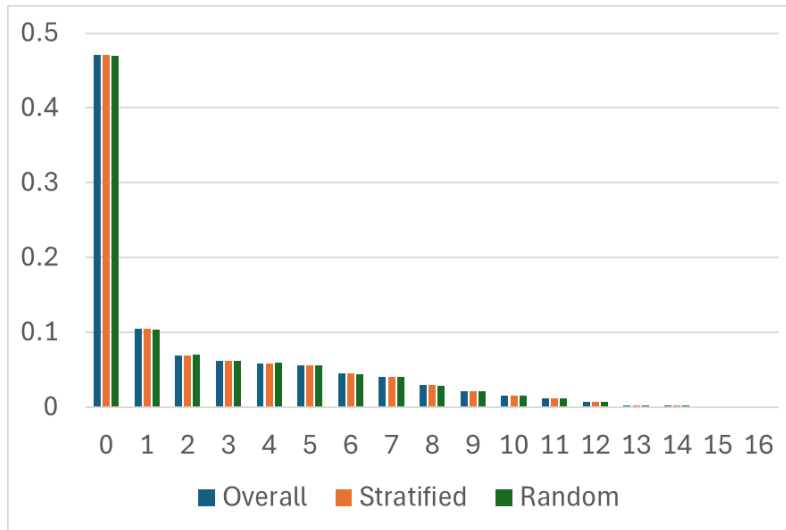


Meaning of chemical descriptors (CDs)	Number of attributes		Attributes
Stoichiometric attributes	6		Ncomp, Comp_L2Norm, Comp_L3Norm, Comp_L5Norm, Comp_L7Norm, Comp_L10Norm
Elemental-property-based attributes	132	Mean (22)	Atomic Number, MendeleevNumber, AtomicWeight, MeltingT, Column, Row, CovalentRadius, Electronegativity, NsValence, NpValence, NdValence, NfValence, NValence, NsUnfilled, NpUnfilled, NdUnfilled, NfUnfilled, NUnfilled, GSvolume_pa, GSbandgap, GSmagmom, SpaceGroupNumber
		Range (22)	
		Dev (22)	
		Max (22)	
		Min (22)	
		Most (22)	
Valence orbital occupation attributes	4		frac_sValence, frac_pValence, frac_dValence, frac_fValence
Ionic compound attributes	3		CanFormIonic, MaxIonicChar, MeanIonicChar

Data distribution



Random vs Stratified sampling



Thank you

