Seeking topological phase transition applying pressure to Ag_3AuSe_2 and Ag_3AuTe_2

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Introduction

- Topological materials, a brand new field

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- Group theory as main tool to determine topological properties

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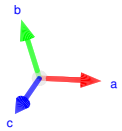
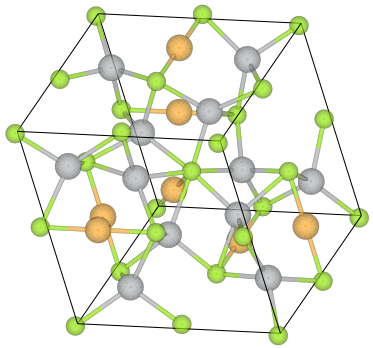
Structure of Ag_3AuSe_2

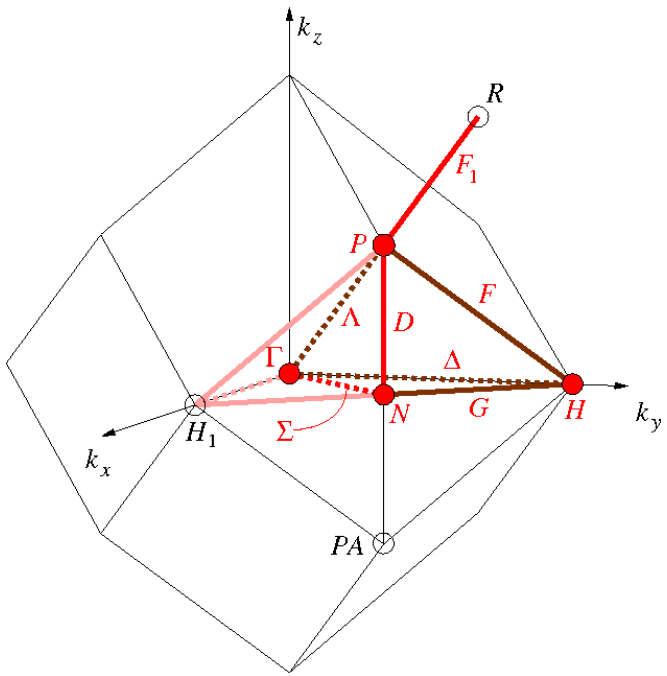




(a) Primitive

(b) Conventional

Brillouin zone of the crystallographic group 214



$$\Gamma - H - N - \Gamma - P - H|P - N$$

Generators of the crystallographic group 214

No.	Symmetry operation(Seitz symbols)
1	$\{E\|0\}$
2	$\{2_{001}\|1/2\ 0\ 1/2\}$
3	$\{2_{010}\|0\ 1/2\ 1/2\}$
4	$\{3^{+}_{111}\|0\}$
5	$\{2_{110}\|3/4\ 1/4\ 1/4\}$
6	$\{1\|1/2\ 1/2\ 1/2\}$

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Main steps

- Choose the approximation for the $E_{XC}(\mathrm{r})$ (LDA or GGA)

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- Choose the approximation for the $E_{XC}(\mathrm{r})$ (LDA or GGA)
- Self consistent calculation $\rightarrow$ Ground state density $n_0(\mathrm{r}) \rightarrow$ $\rightarrow$ Effective Hamiltonian $H_{eff}(\mathrm{r})$
- Calculate energy bands and Bloch wavefunctions:

$$H_{eff}(\mathrm{r})\psi_{n,\mathrm{k}}(\mathrm{r}) = \varepsilon_n(\mathrm{k})\psi_{n,\mathrm{k}}(\mathrm{r}) \tag{1}$$

$$\psi_{n\mathrm{k}}(\mathrm{r}) = e^{i\mathrm{kr}}u_{n\mathrm{k}}(\mathrm{r}) \; ; \; u_{n\mathrm{k}}(\mathrm{r}+\mathrm{R}) = u_{n\mathrm{k}}(\mathrm{r}) \tag{2}$$

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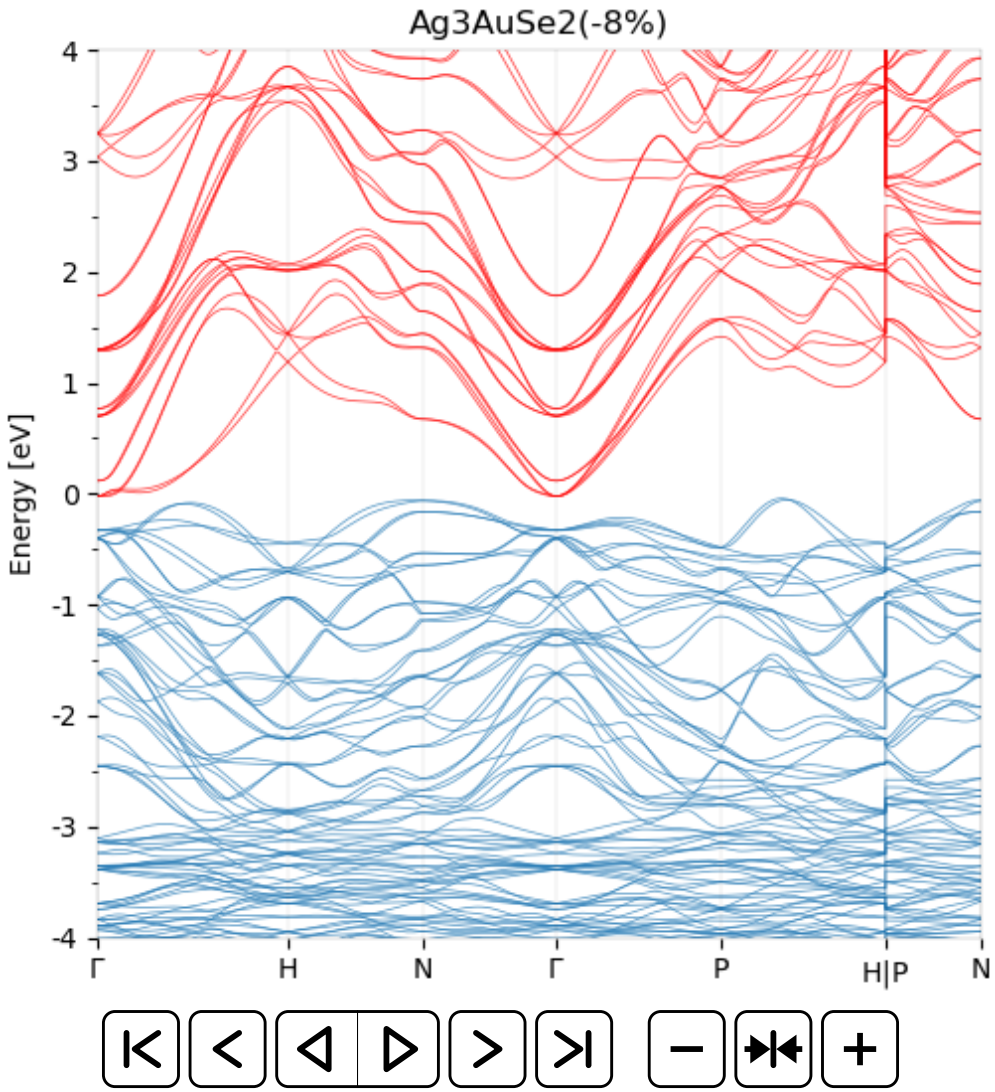
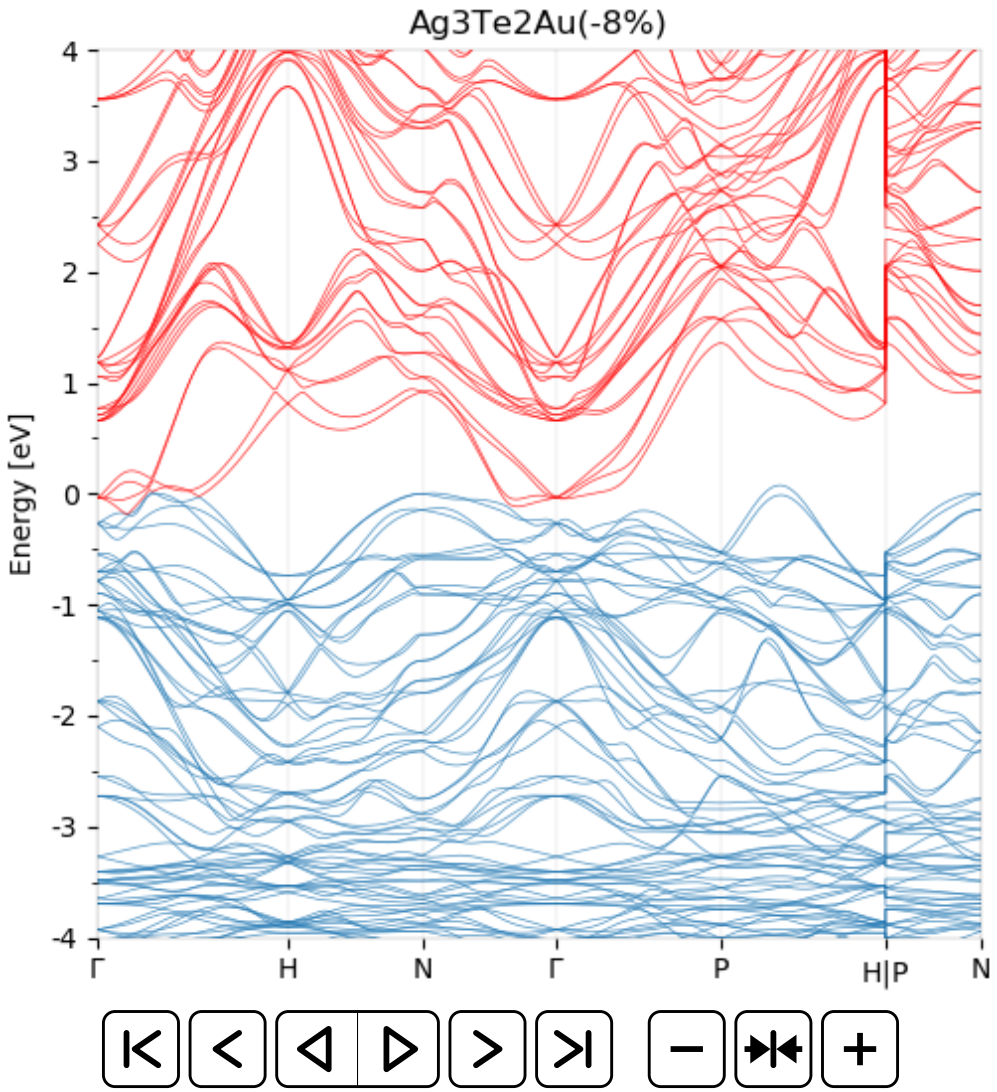
Applying pressure to Ag_3AuSe_2



Applying pressure to Ag_3AuTe_2



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Decomposition of representations

Decomposition into irreducible representations:

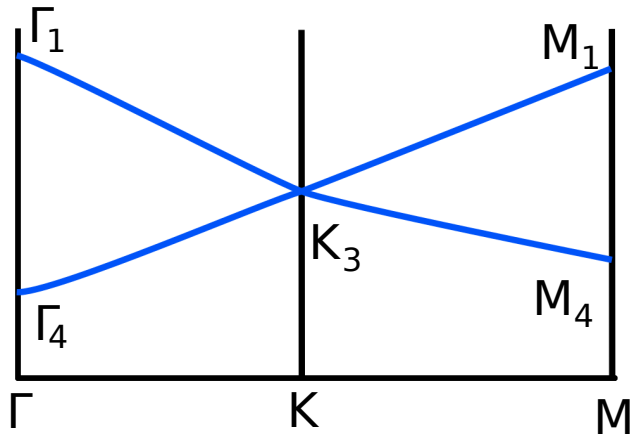
$$(\rho \uparrow G) \downarrow G_k \cong \bigoplus_i m_i^k \sigma_i^k \tag{3}$$

Magic formula:

$$m_i^k = (\rho|\sigma_i^k) = \frac{1}{g} \sum_{t \in G_k} \chi[\sigma_i^k(t)] \overline{\chi[\rho(t)]} \tag{4}$$

Band representation

- A band representation is a way to encode the symmetry information of the bands



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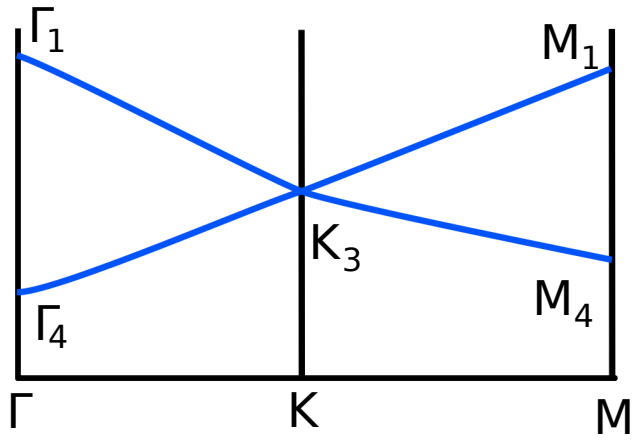

- BR $= (\Gamma_1;\ \Gamma_2;\ \Gamma_3;\ \Gamma_4;\ \mathrm{K}_1;\ \mathrm{K}_2;\ \mathrm{K}_3;\ \mathrm{M}_1;\ \mathrm{M}_2;\ \mathrm{M}_3;\ \mathrm{M}_4)$

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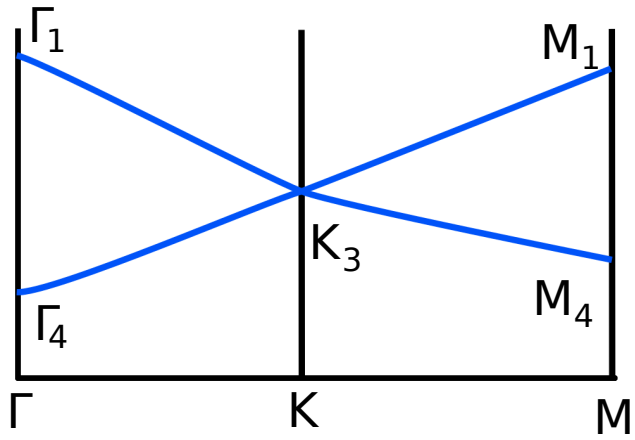

- BR = (Γ_1; Γ_2; Γ_3; Γ_4; K_1; K_2; K_3; M_1; M_2; M_3; M_4)
- BR = (1,0,0,1,0,0,1,1,0,0,1)

Elementary band representation

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- Decompose the BR into EBR :
  $\mathrm{BR} = \sum_i c_i EBR_i$
- Then there are three cases :
  1. Trivial bands : all c_i positive integers
  2. Weak topological bands : one or more c_i negative integer
  3. Strong topological bands : one or more fractional c_i

Vasp2trace analysis

Both trivial insulators except:

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- Ag_3AuTe_2 is ESFD when $1\% \leq \gamma \leq 5\%$

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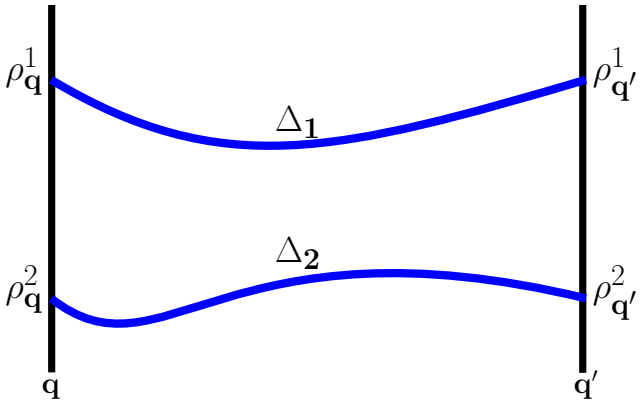
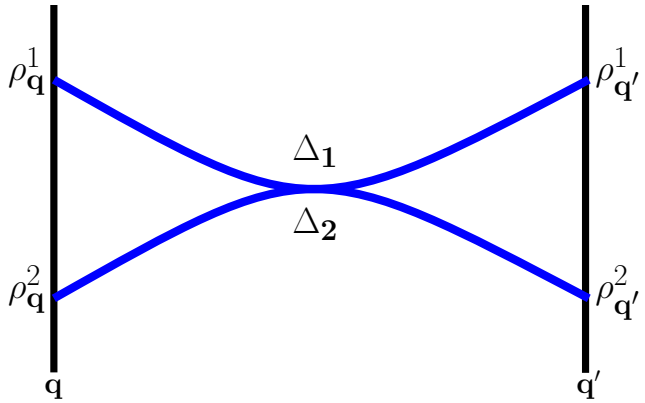
- Ag_3AuSe_2 is ESFD when $1\% \leq \gamma$

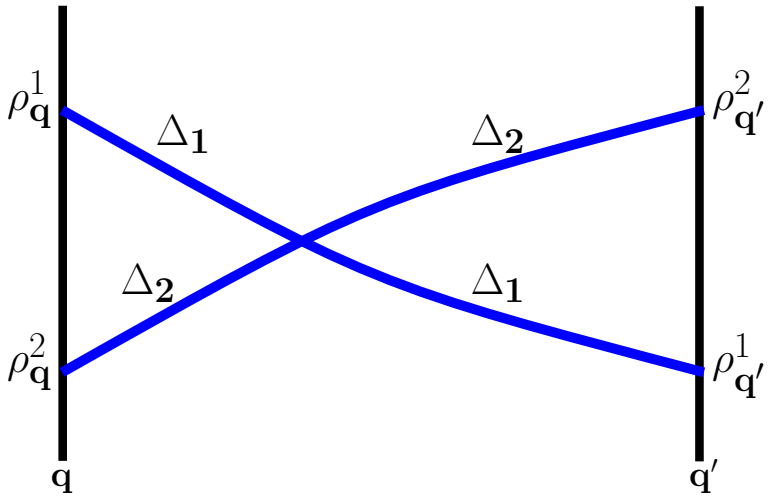
Enforced crossing



(a) No crossing



(b) Accidental crossing



(c) Enforced crossing

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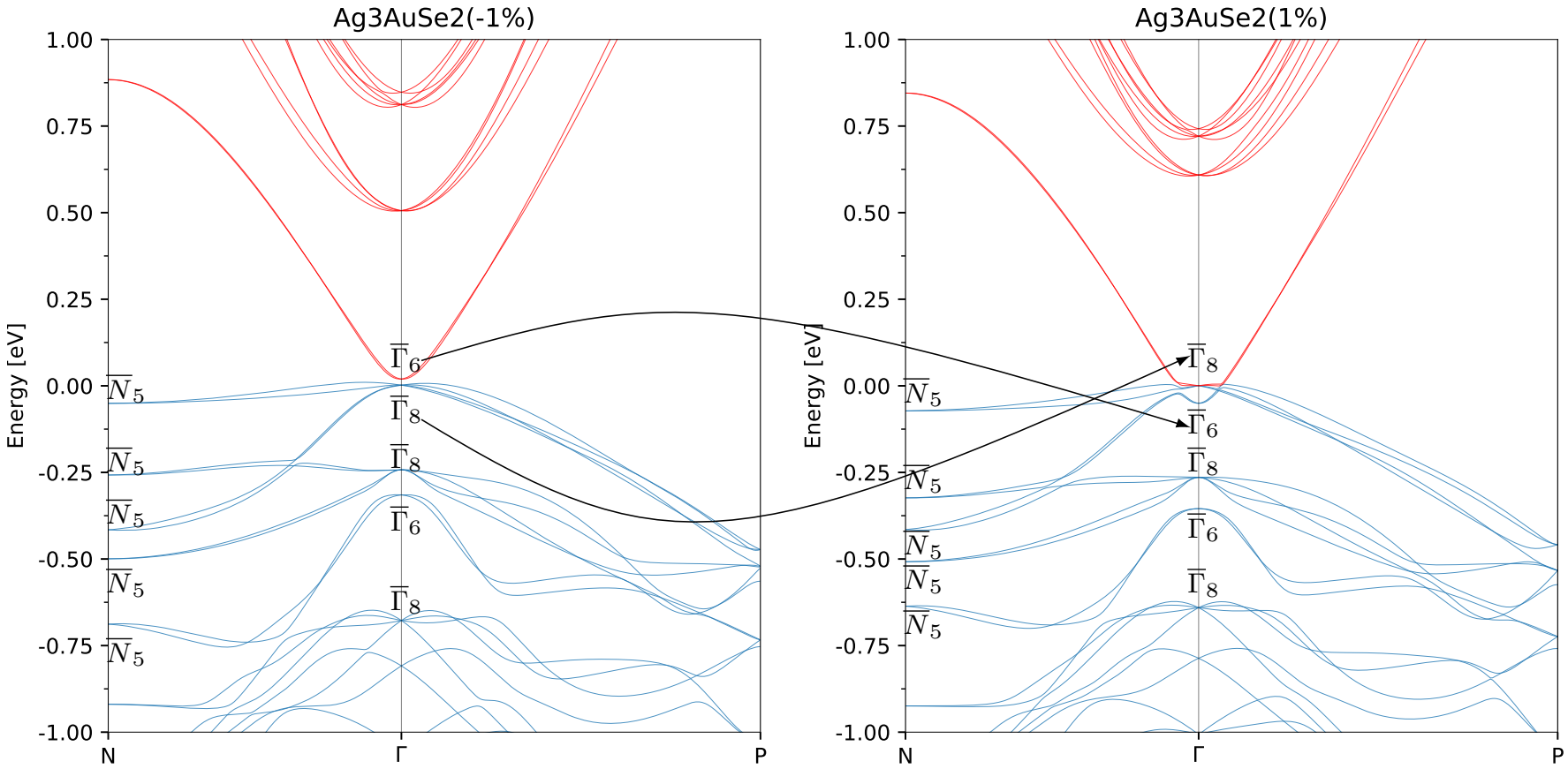

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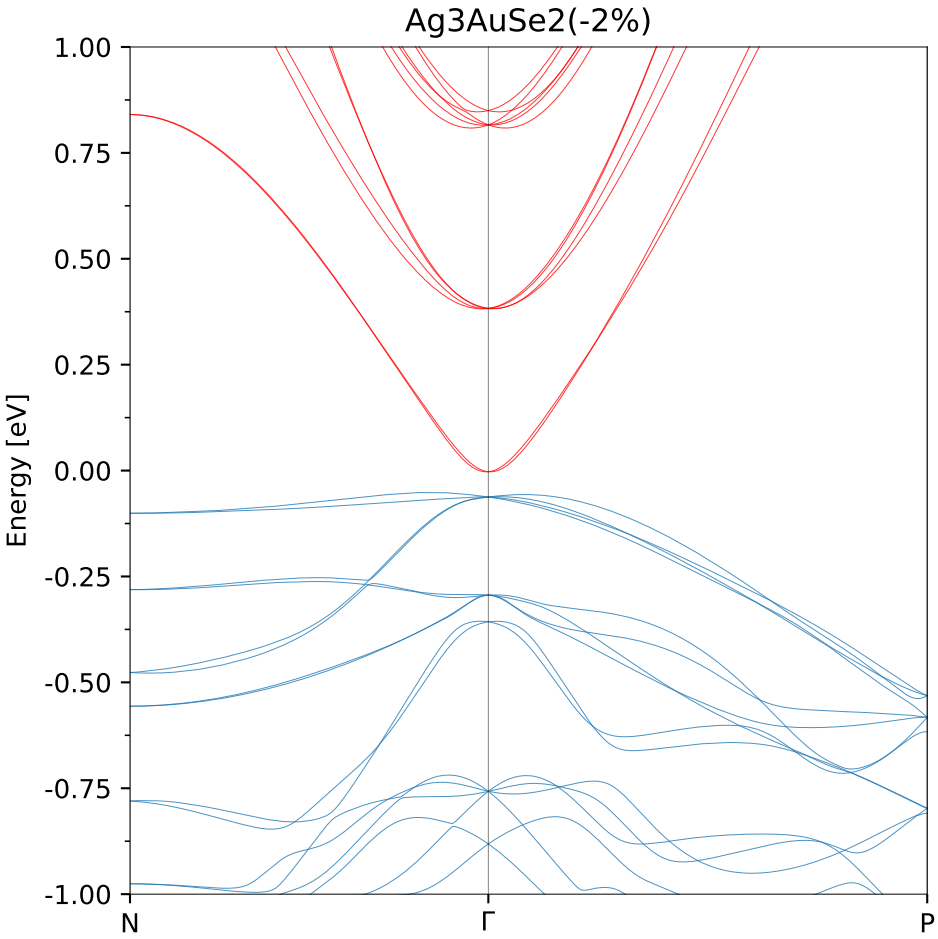

Feasibility:

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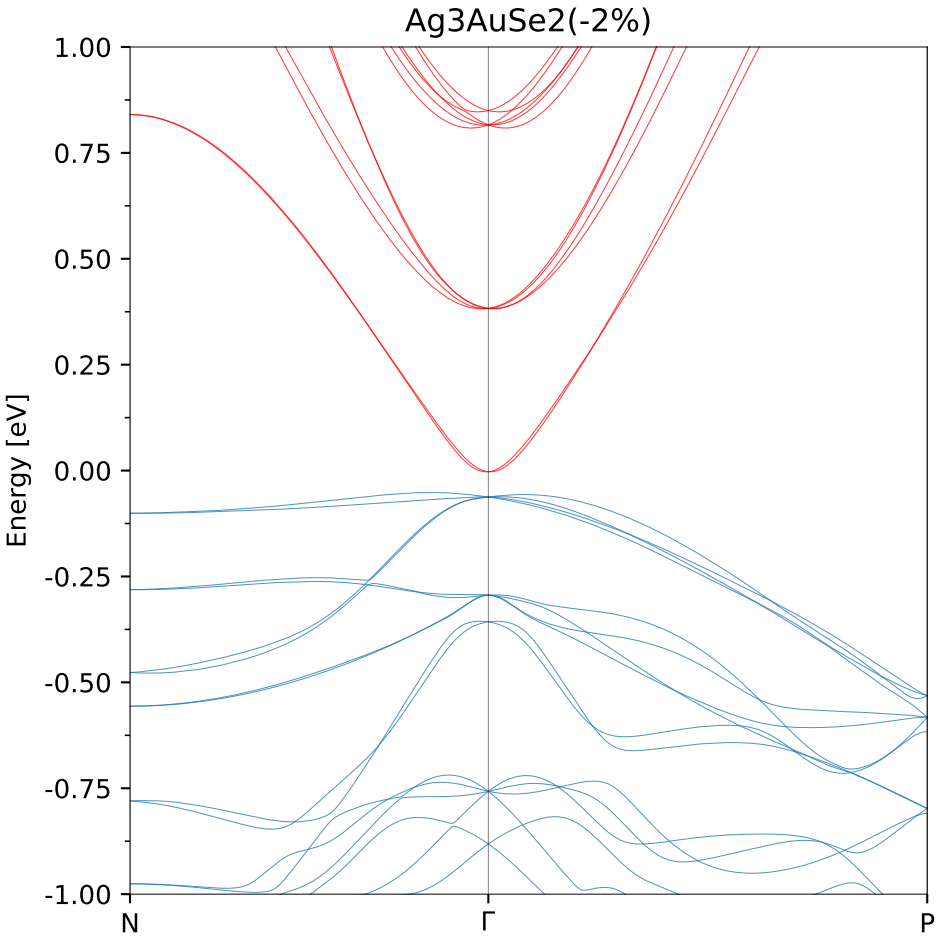

Feasibility:

1. Band gap of order $\sim meV$

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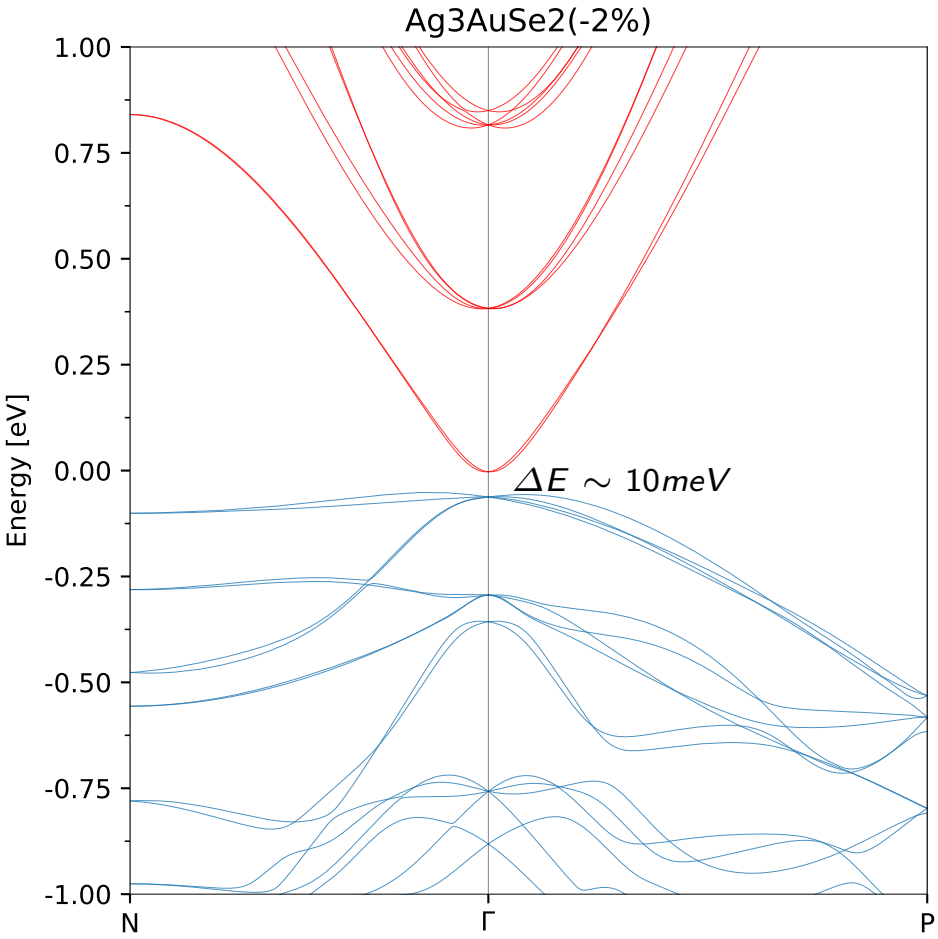

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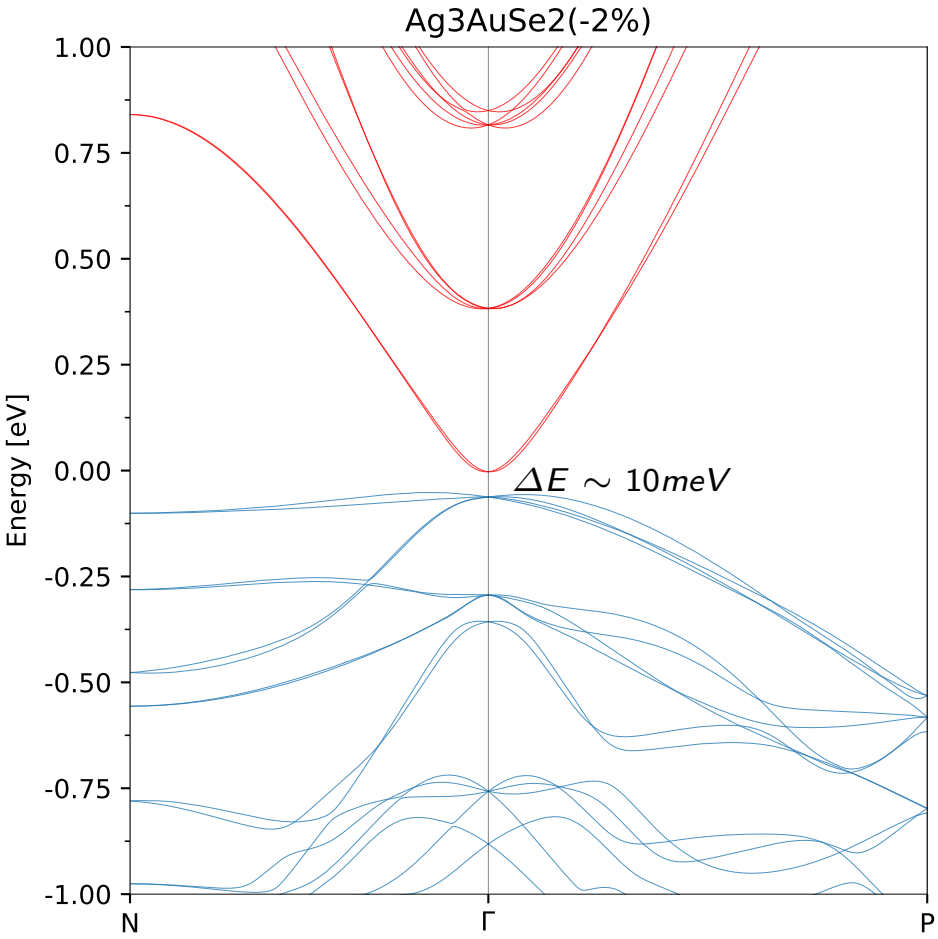

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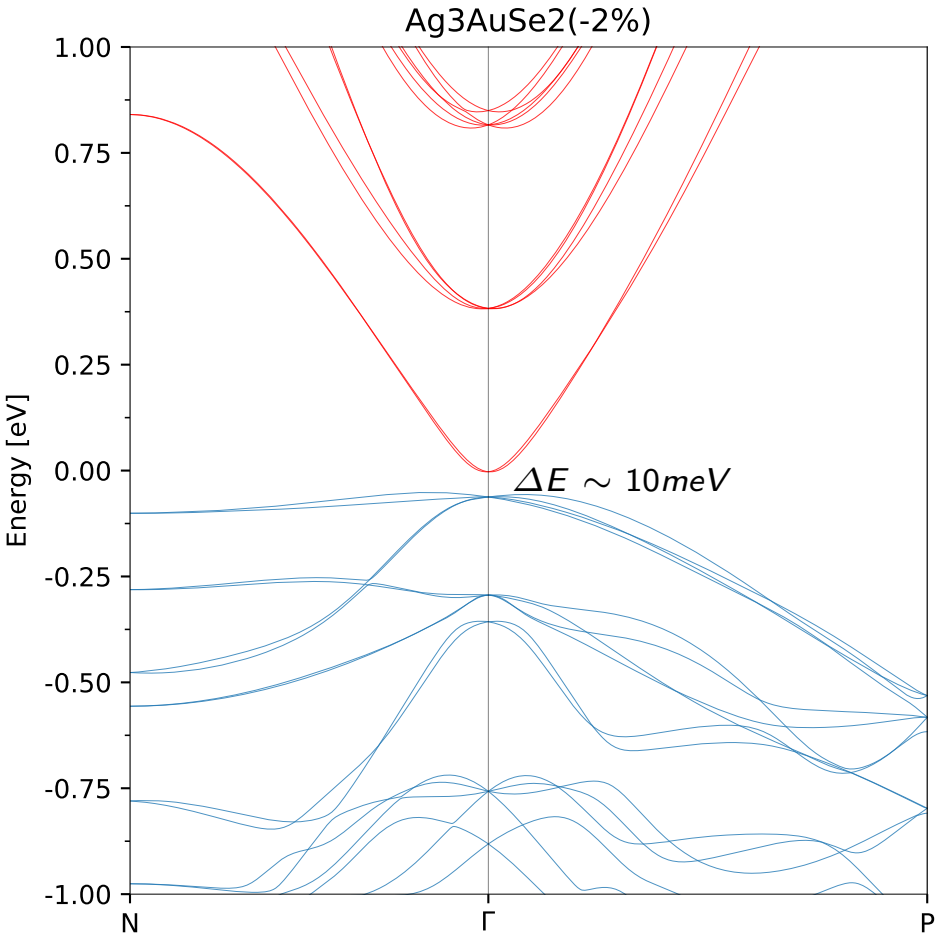

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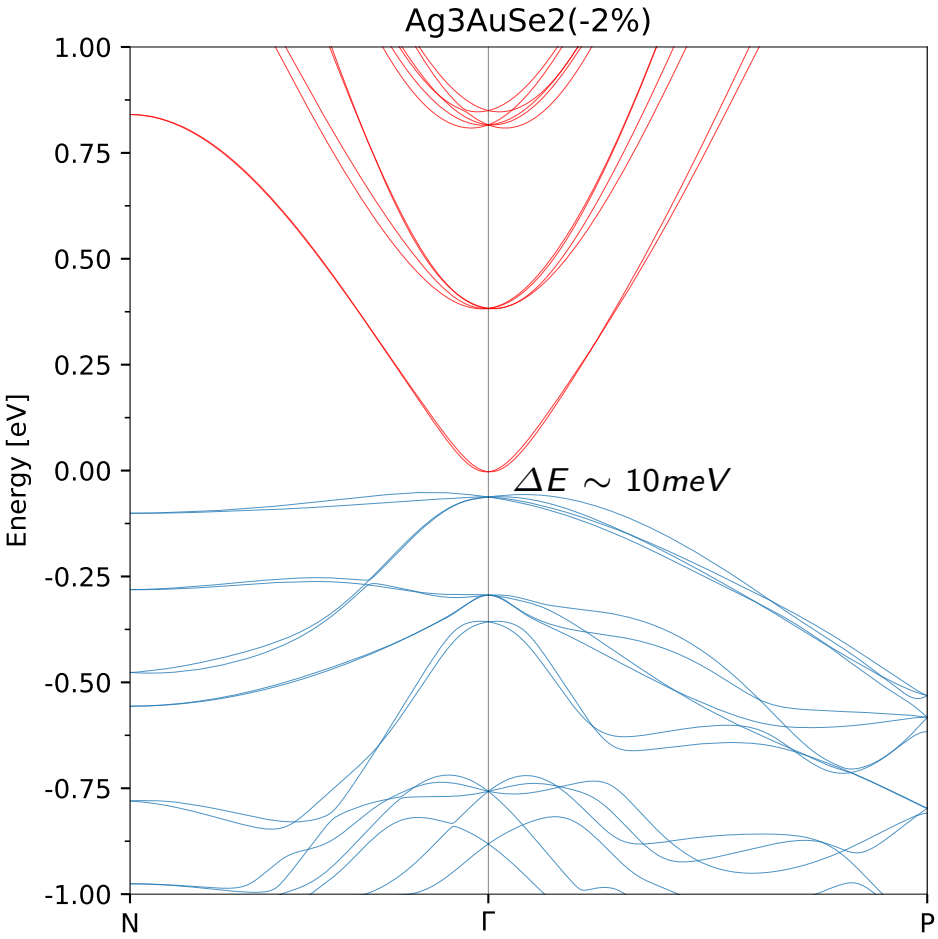

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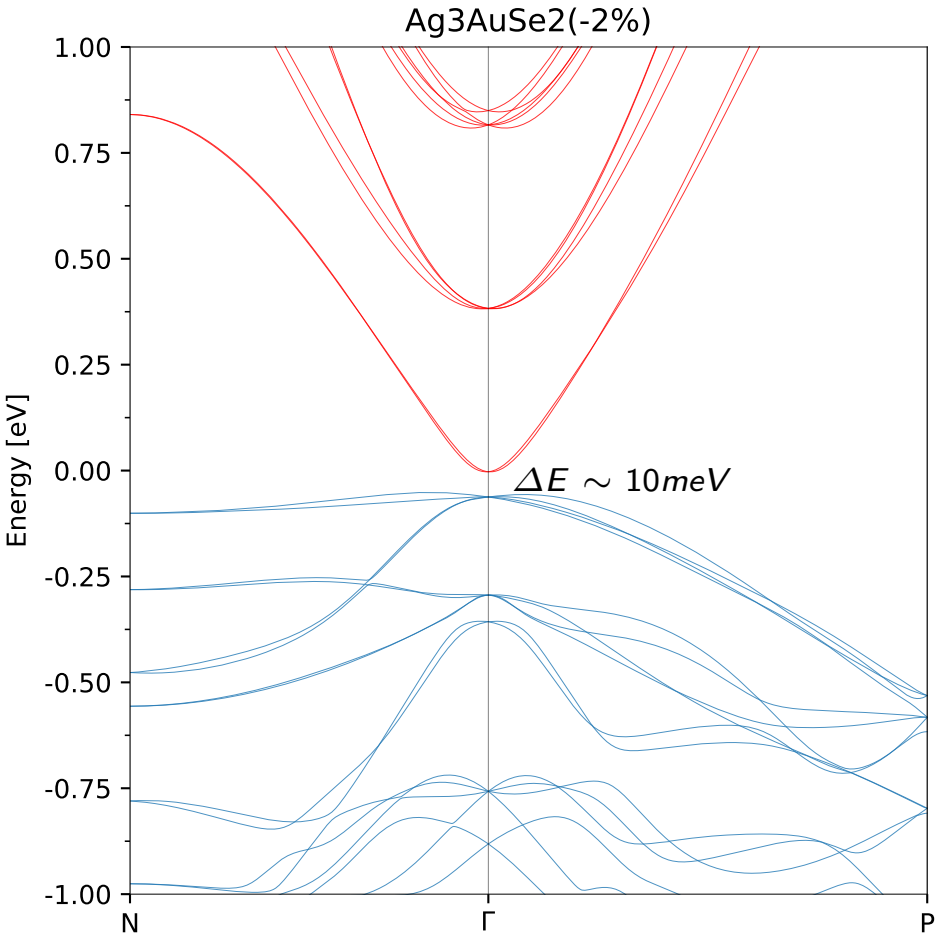

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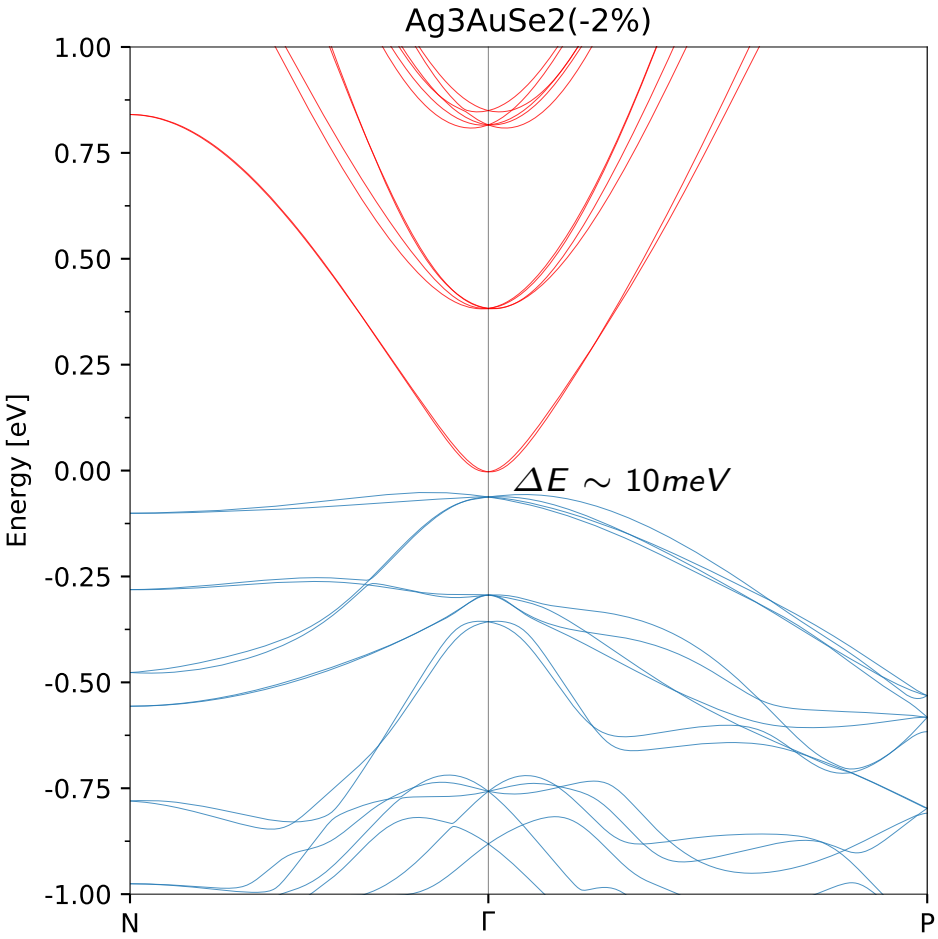

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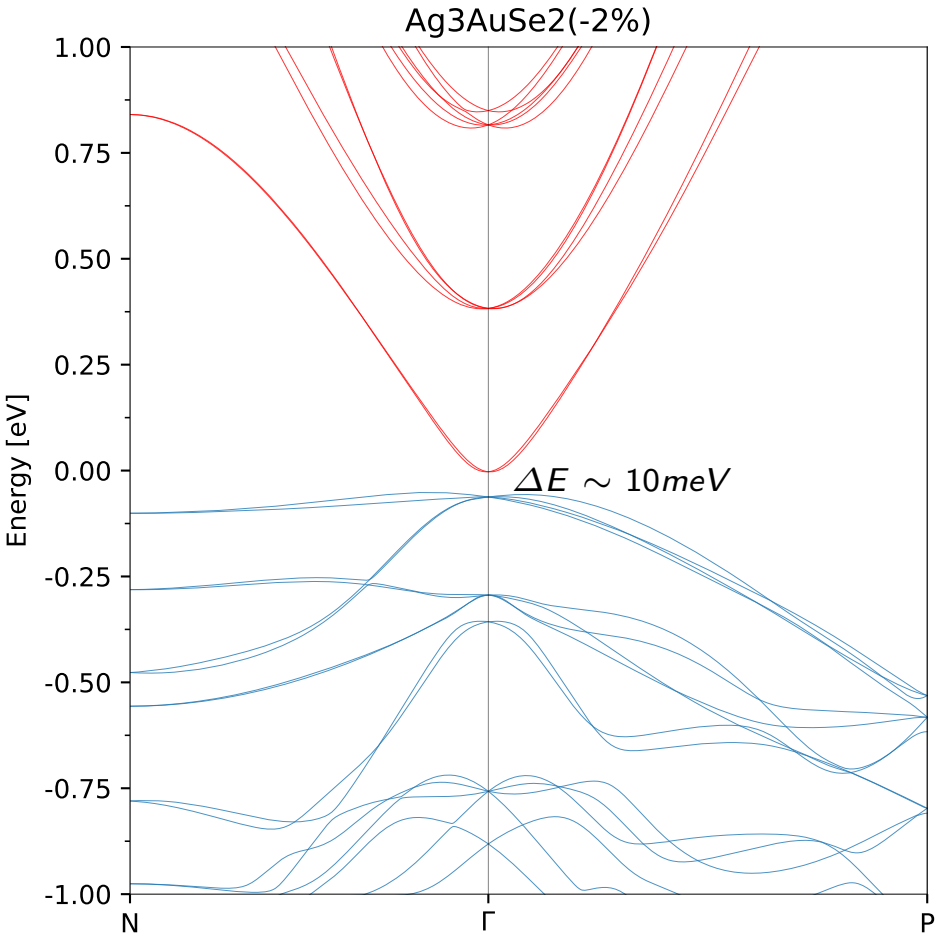

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   Ag_3AuSe_2 is an already studied mineral

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