Trabajo Fin de Grado
Grado en Químicas
Curso 2025-2026

SIMULACIÓN DE MATERIALES

DIEGO GARCÍA DORADO

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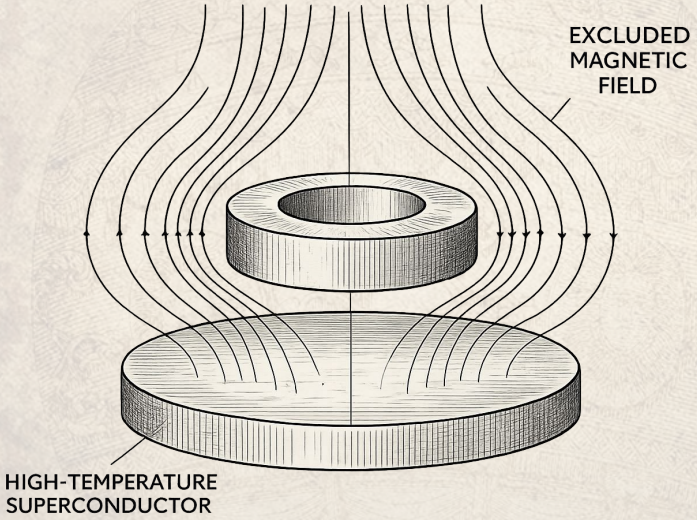
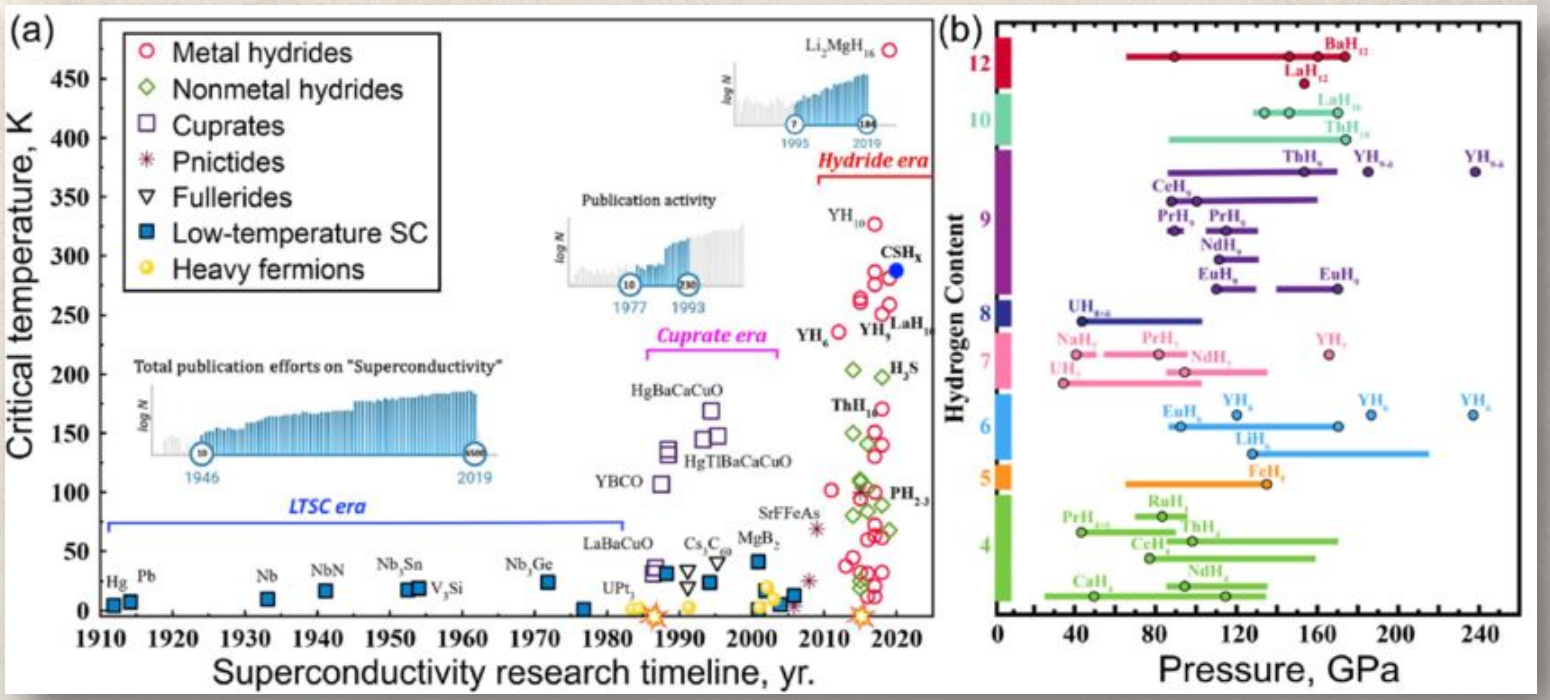
DEPARTAMENTO DE QUÍMICA FÍSICA

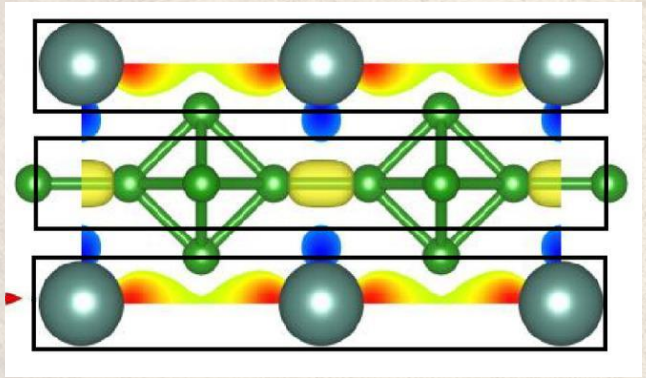
SUPERCONDUCTIVITY AND HYDRIDES

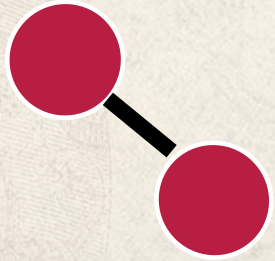




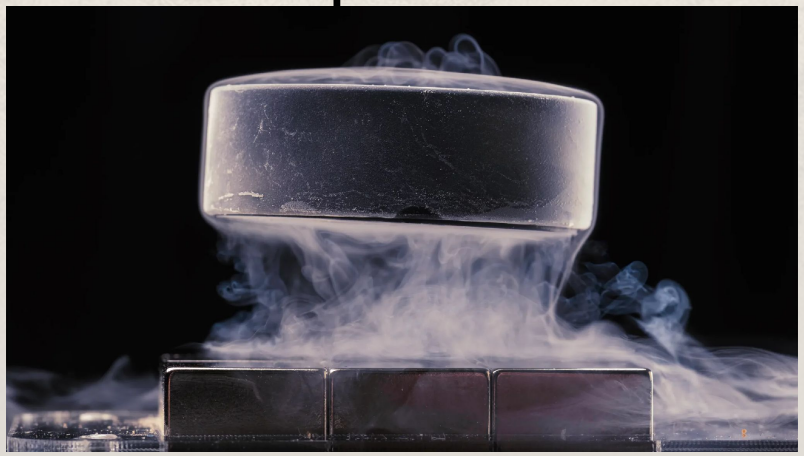
Hydrides → Highest Critical Temperature

CHEMICAL BONDING IN SUPERCONDUCTORS?





How can we improve the critic temperature?

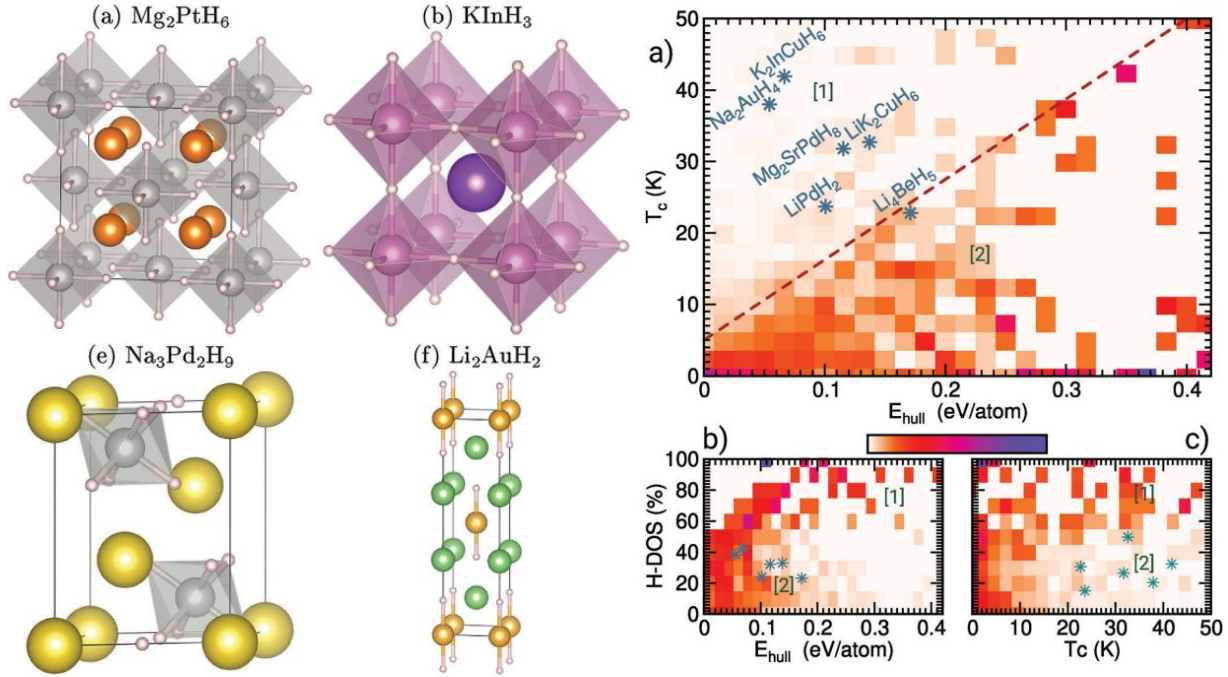


ADVANCED FUNCTIONAL MATERIALS

Searching Materials Space for Hydride Superconductors at Ambient Pressure

Tiago F. T. Cerqueira, Yue-Wen Fang, Ion Errea, Antonio Sanna, and Miguel A. L. Marques**

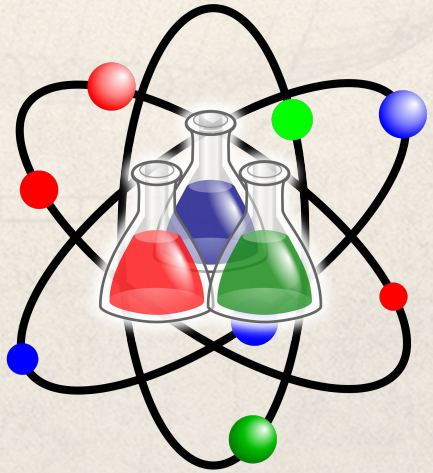
19 June 2024

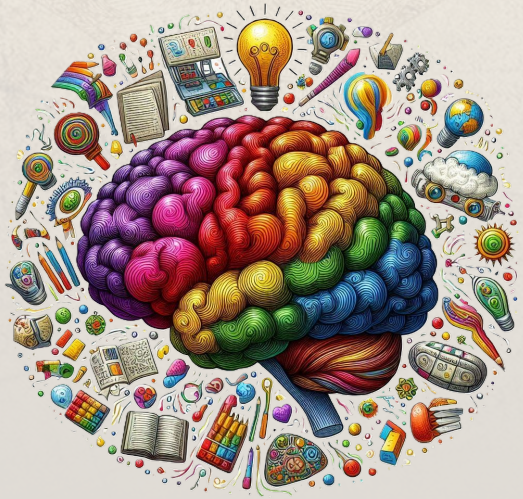


OBJETIVOS

Objetivos científicos

- Conocer el enlace químico en hidruros
- Estudiar los orbitales cristalinos de la red
- Comprender la relación con Tc

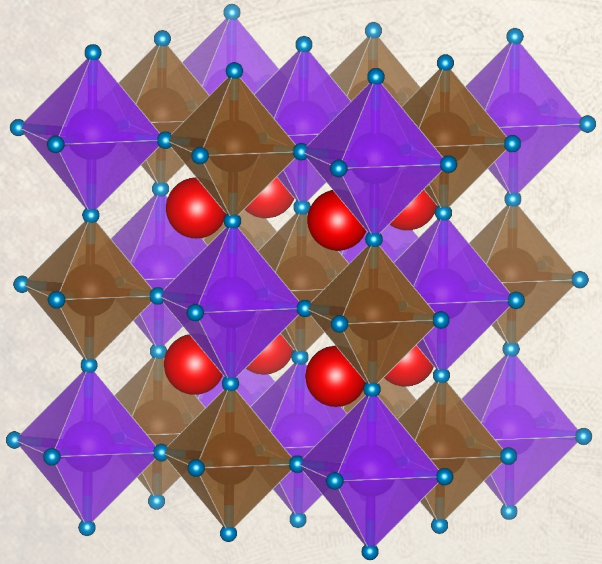




Objetivos de Aprendizaje

- Desarrollo de un trabajo científico.
- Computación química basada en DFT
- Análisis de enlace químico

PEROVSKITAS DE HIDRURO SM_2TMH_6

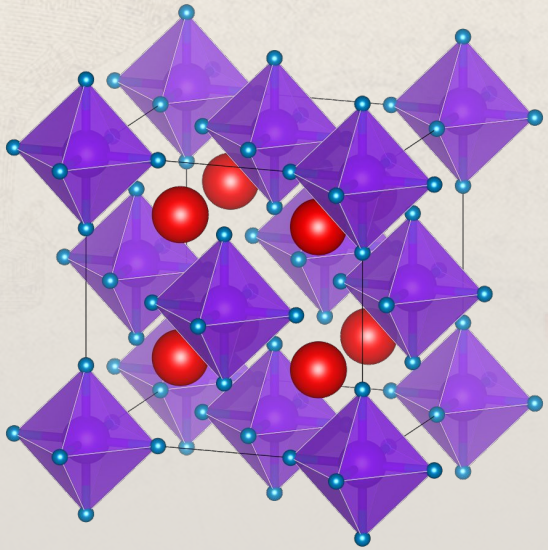


Grupo Fm-3m

TM (4a)

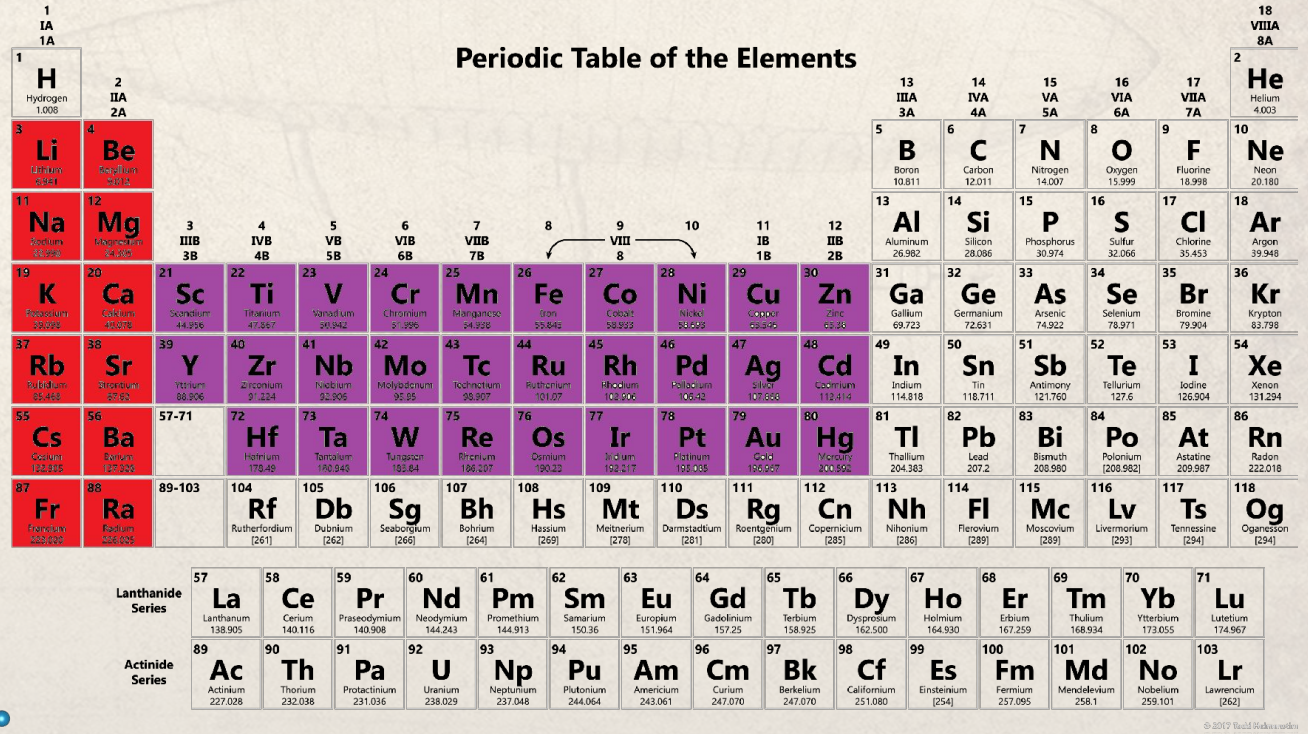
SM(8c)

H(24e)



Estructura

SM_2TMH_6



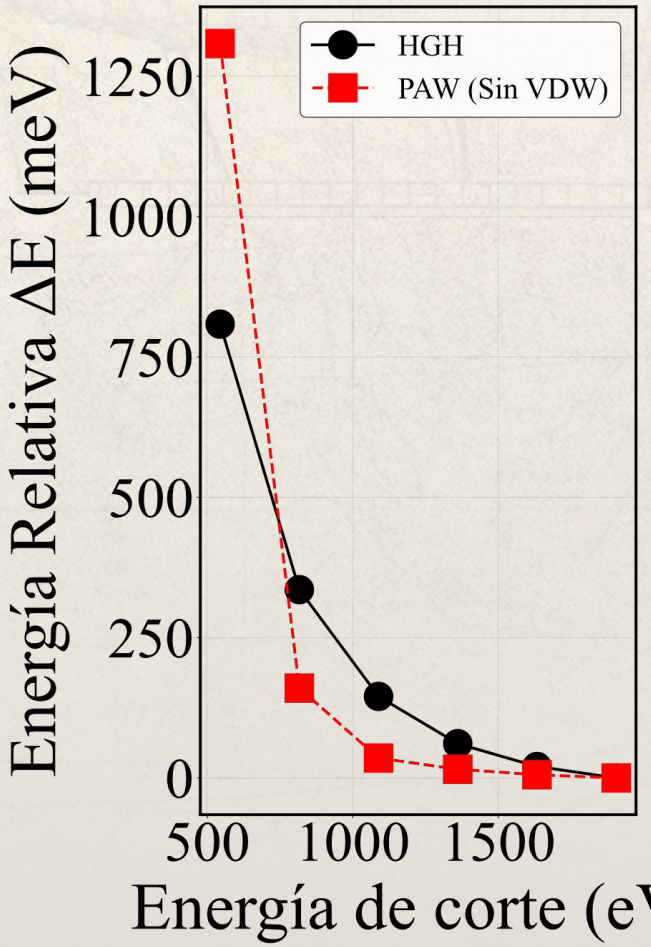
Estructura	Tc(K)
Mg_2PdH_6	63,8
Na_2AgH_6	46,1
Mg_2RhH_6	53,8
Mg_2IrH_6	59,4

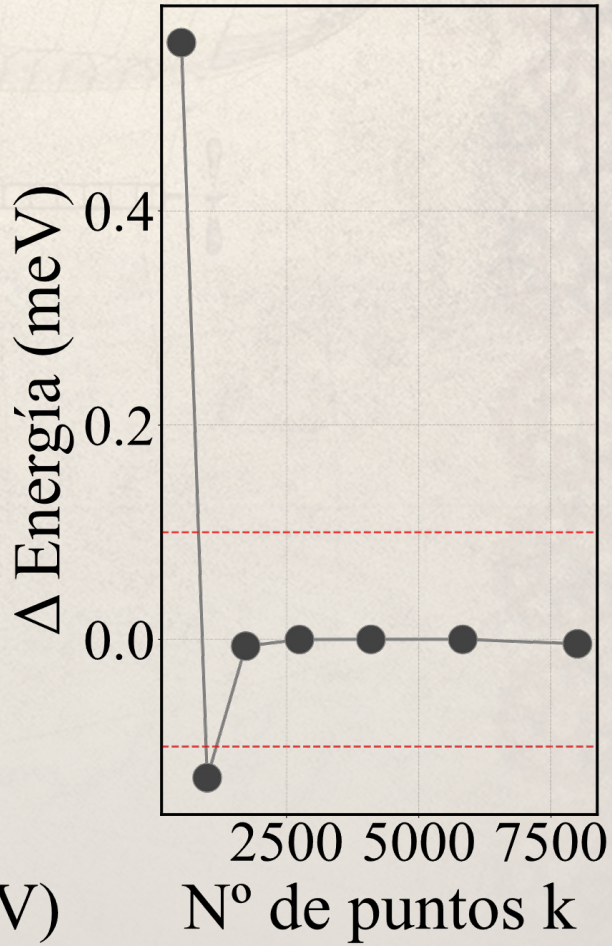
DETALLES COMPUTACIONALES

- Cálculos DFT con PBEsol y PAW
- 15 Estructuras SM_2IrH_6 estudiadas
- Buen acuerdo con la bibliografía:

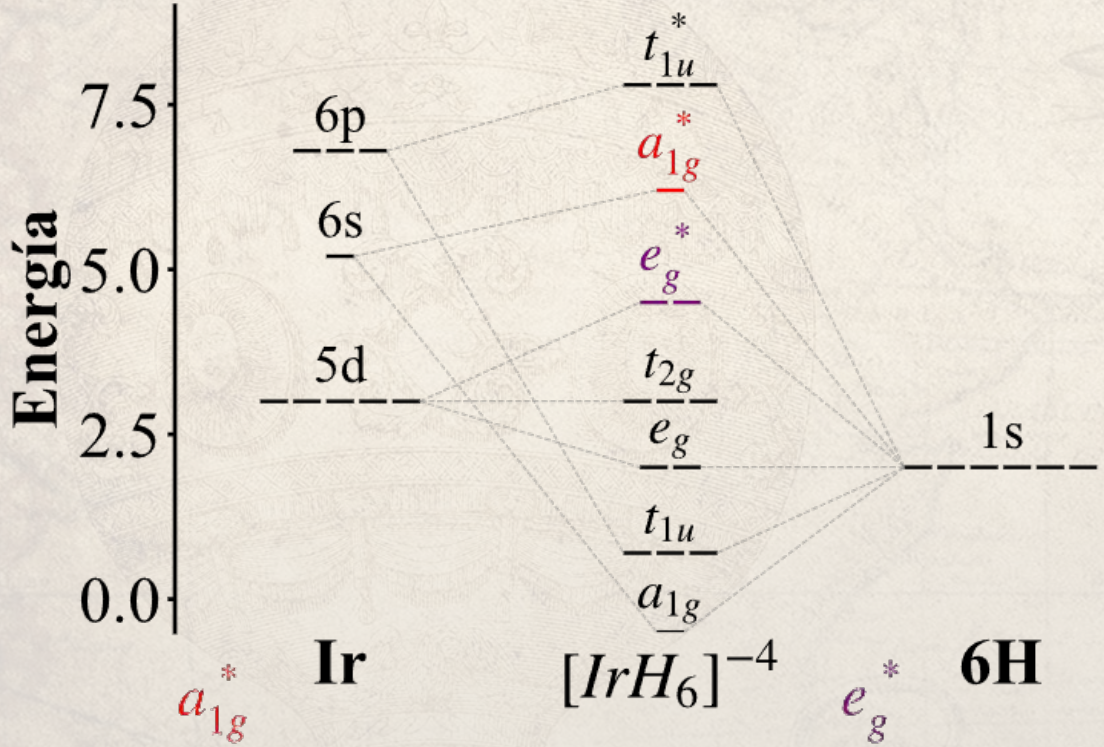
  Mg_2IrH_6 a= 6,66 (Å) Ca_2IrH_6 a=7,20 (Å)

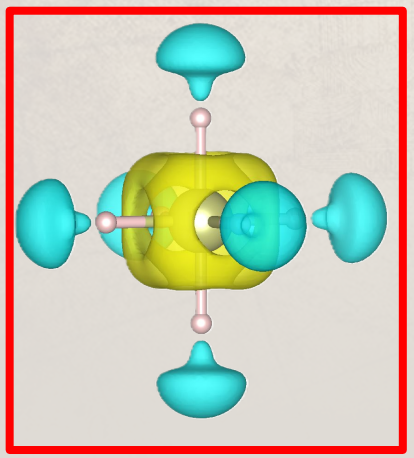
SM	a(Å)	SM	a(Å)	SM	a(Å)
Be_2	5,93	AlLi	6,27	AlSr	7,25
Mg_2	6,50	AlNa	6,54	SrY	7,29
Ca_2	7,07	AlK	7,09	SrSc	7,06
Sr_2	7,46	AlRb	7,36	Sc_2	6,64
Ba_2	7,89	AlCa	7,02	Y_2	7,02

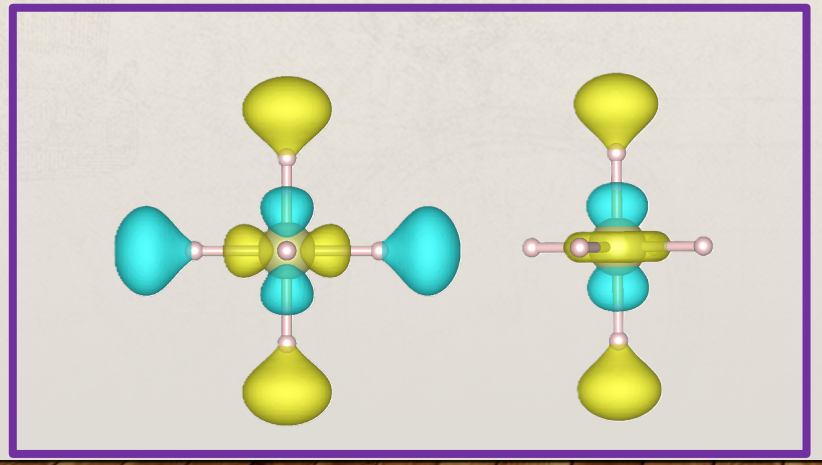


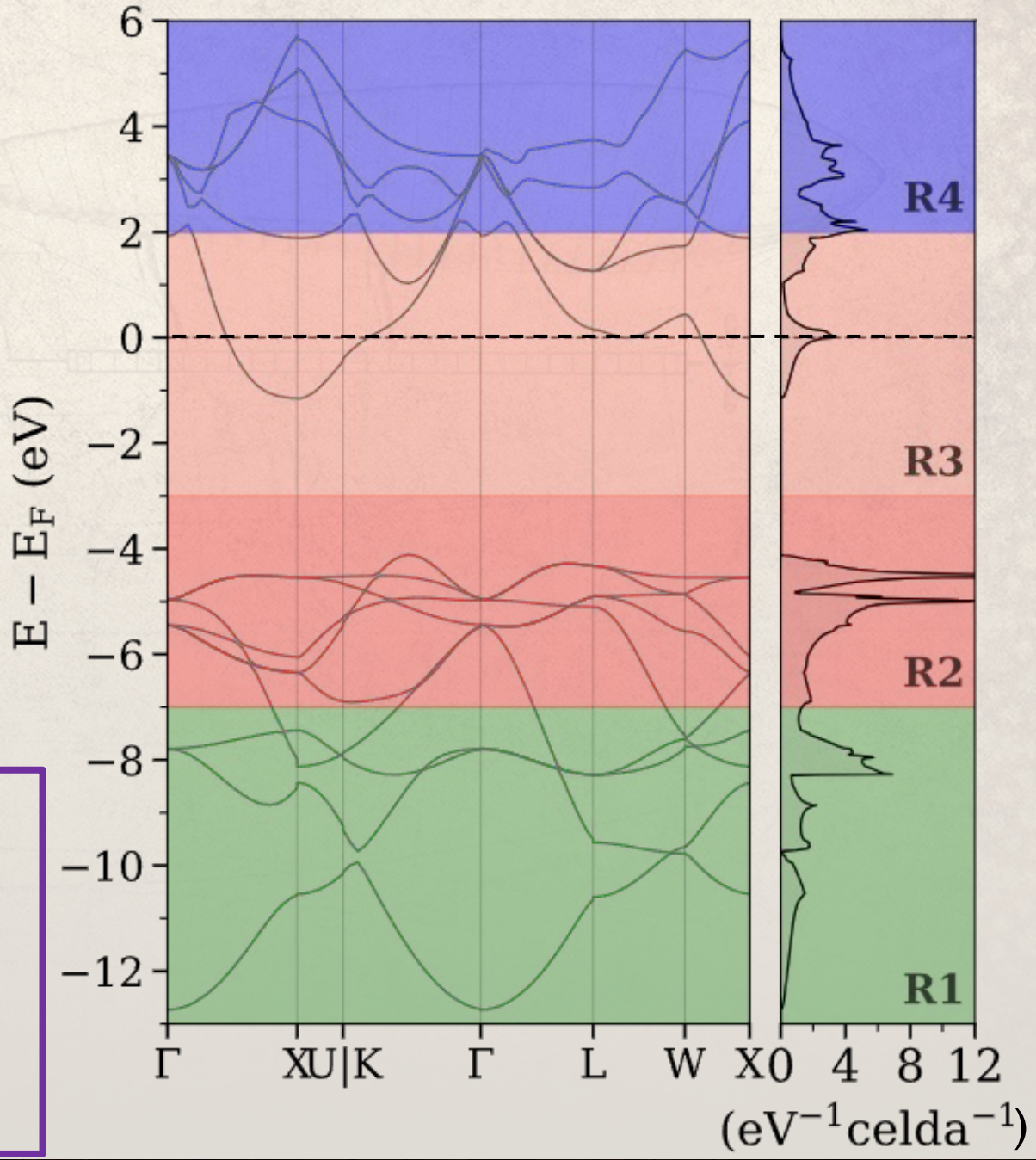


ESTUDIO DEL Mg_2IrH_6

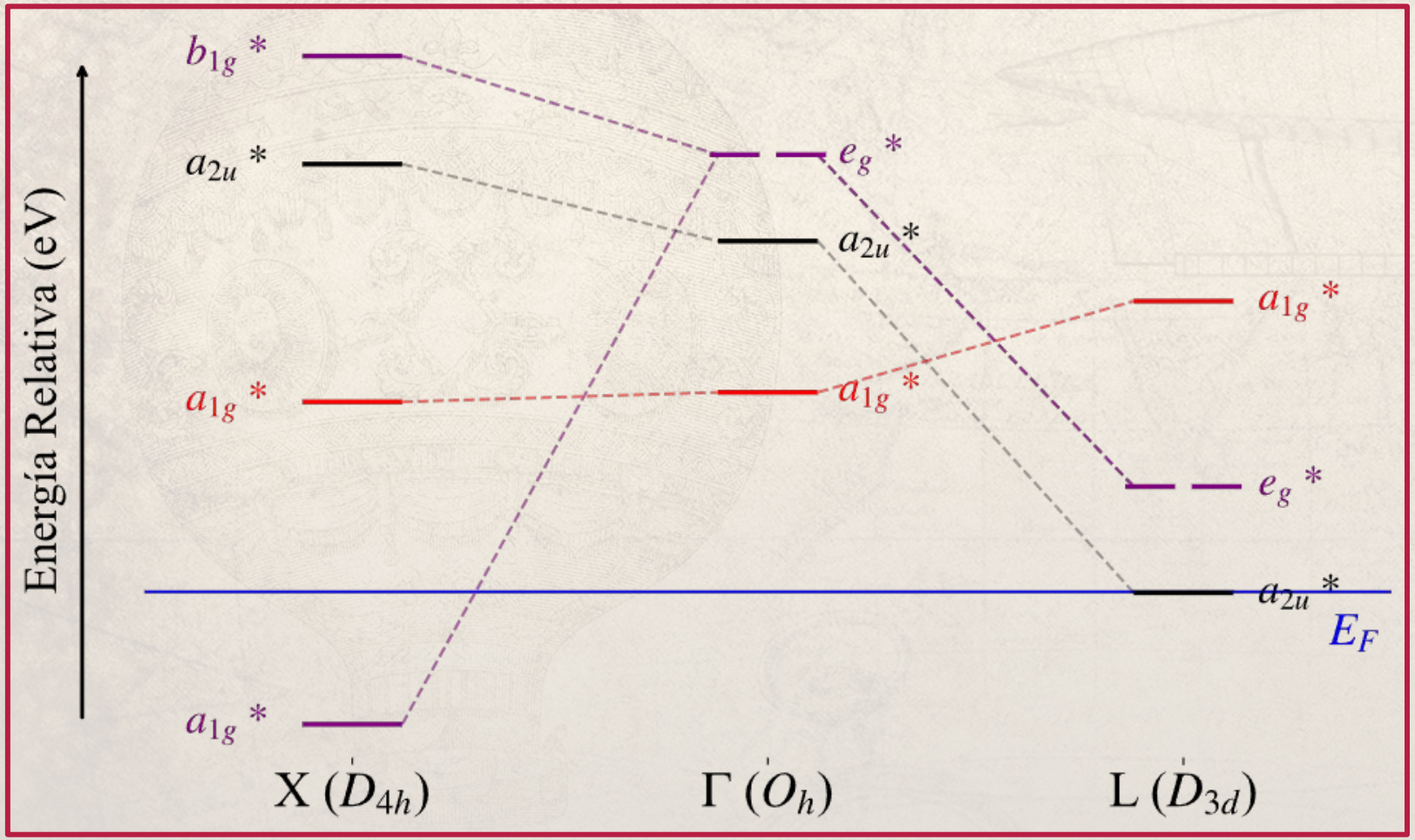




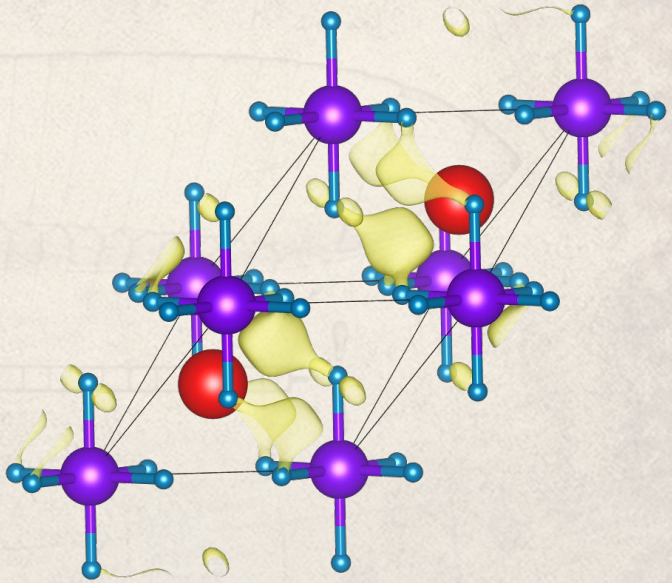




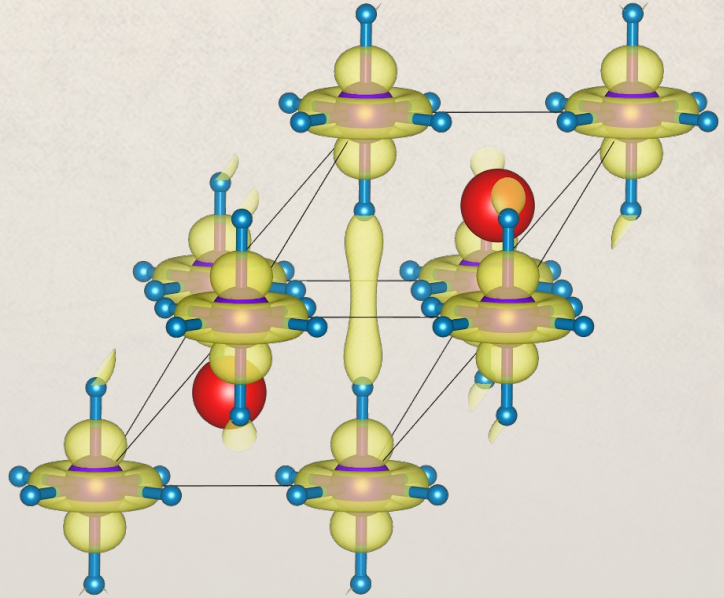
SIMETRÍA DE LOS ORBITALES



L

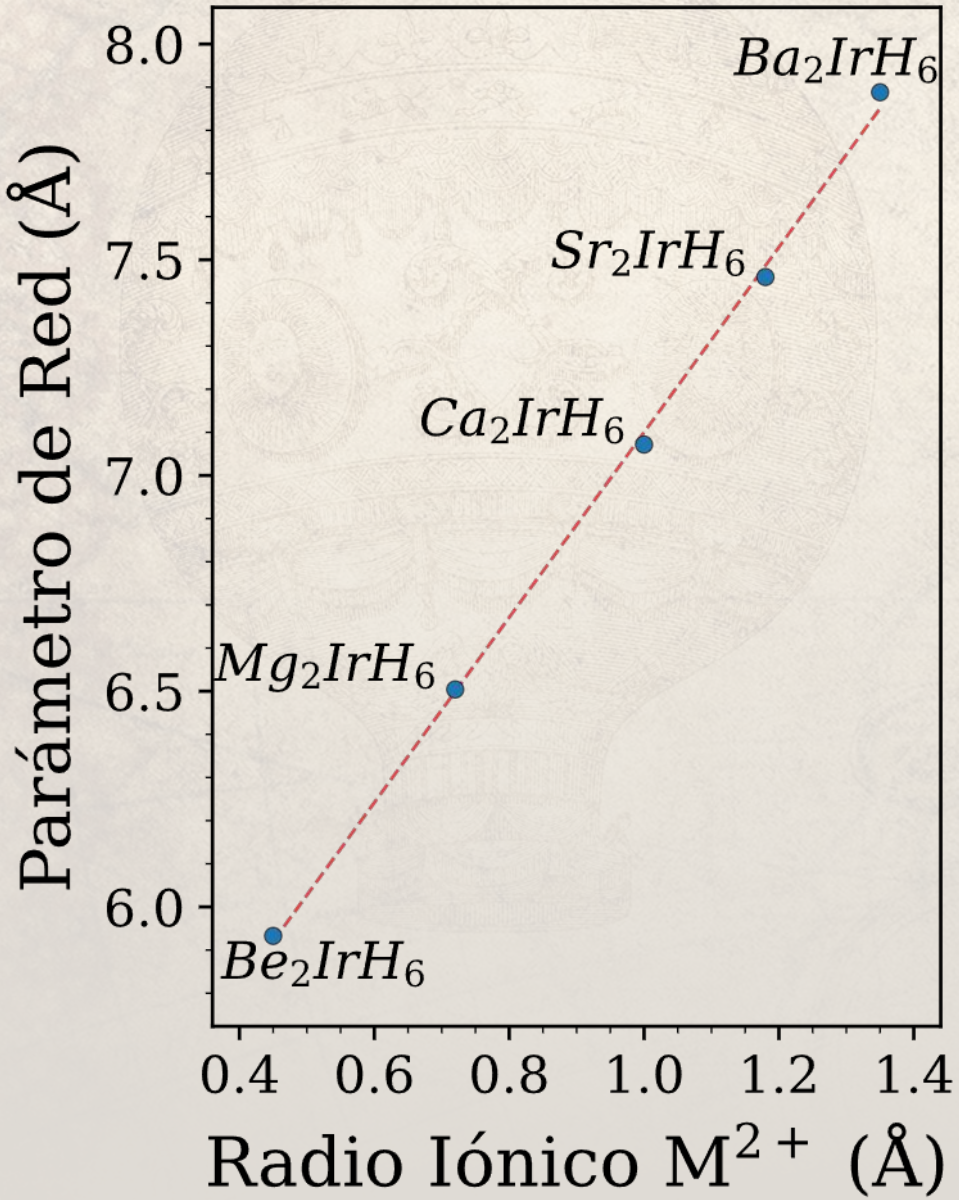


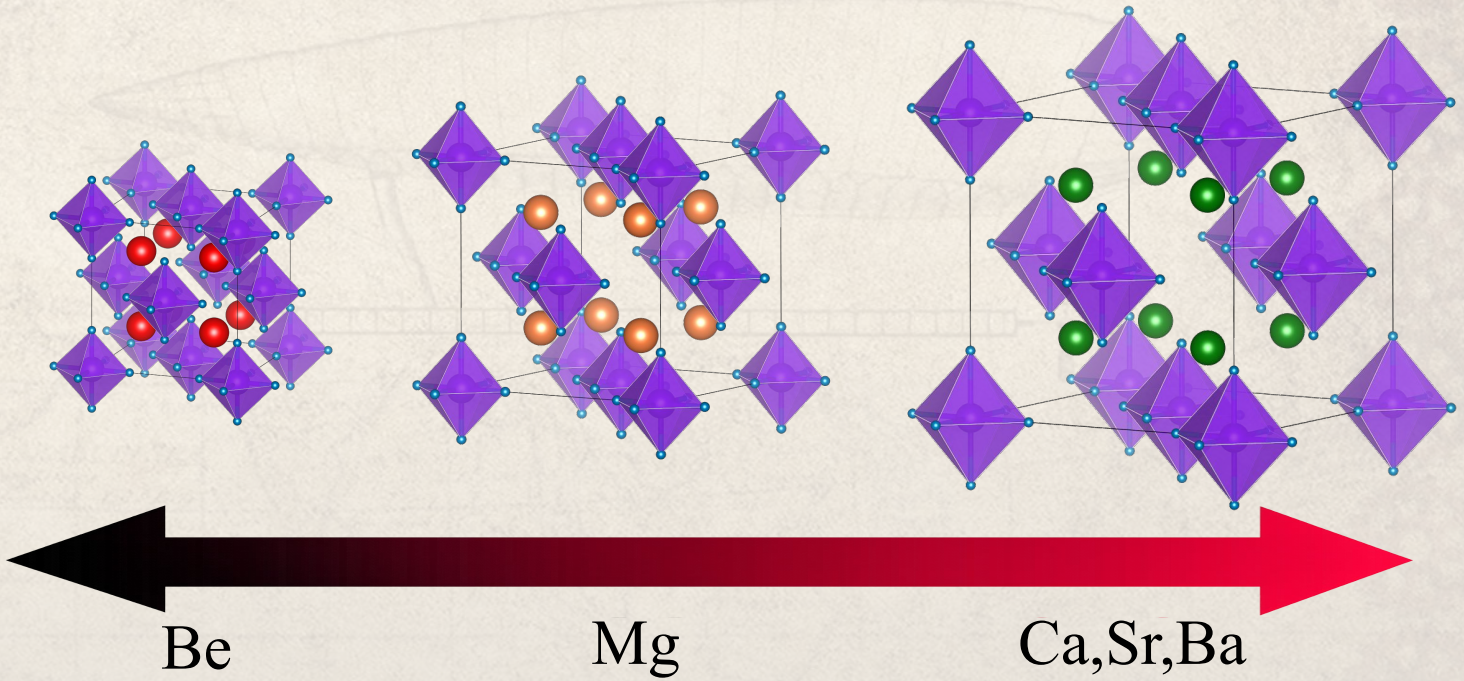
X



Desdoblamientos de los niveles energéticos en relación a la fase del sistema

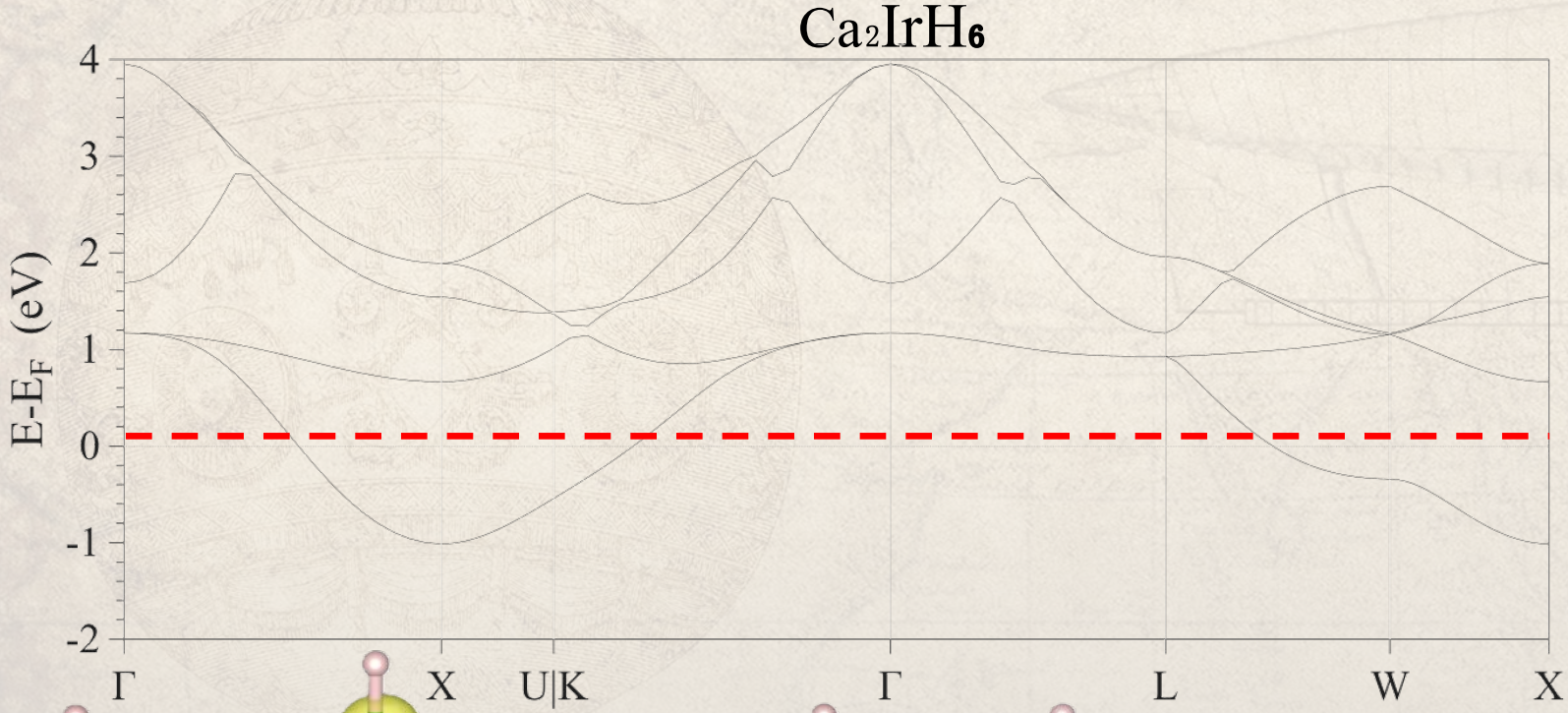
PRESIÓN QUÍMICA

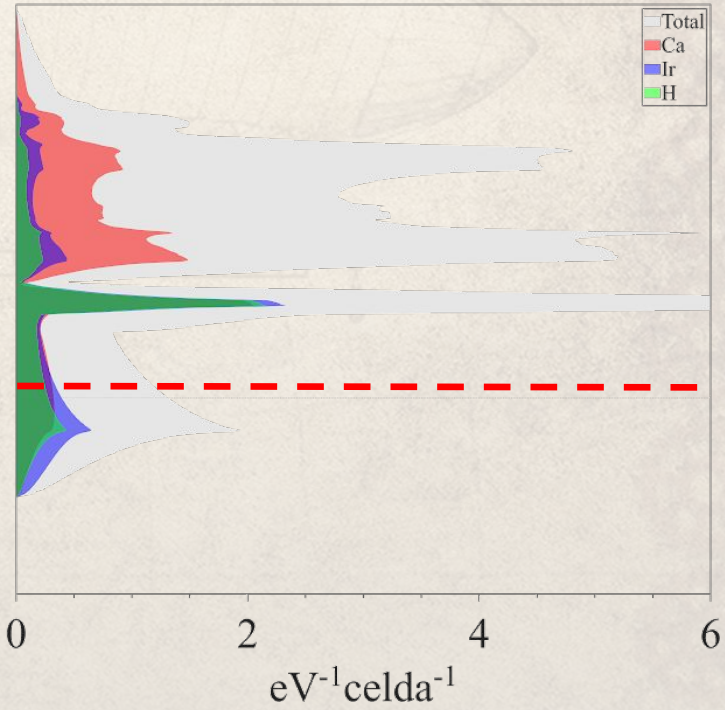


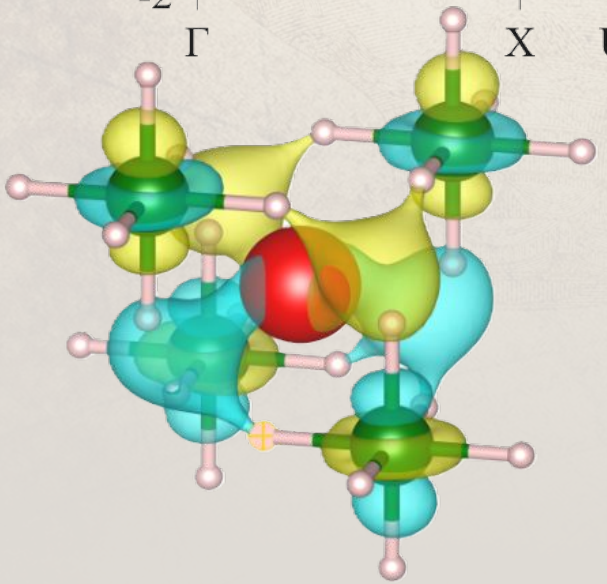


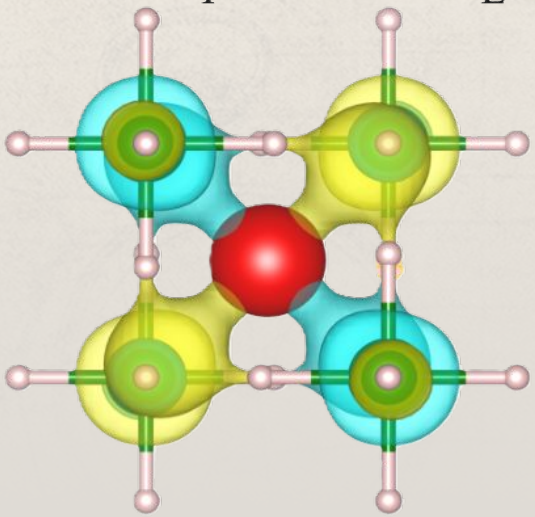
Estructuras	Ir-H	M-H	H-H	a(Å)
Be_2IrH_6	1,69	2,11	1,80	5,93
Mg_2IrH_6	1,71	2,30	2,17	6,50
Ca_2IrH_6	1,71	2,50	2,42	7,07
Sr_2IrH_6	1,71	2,64	2,86	7,46
Ba_2IrH_6	1,71	2,84	3,24	7,89

ORBITALES d Y CARGAS DEL SISTEMA



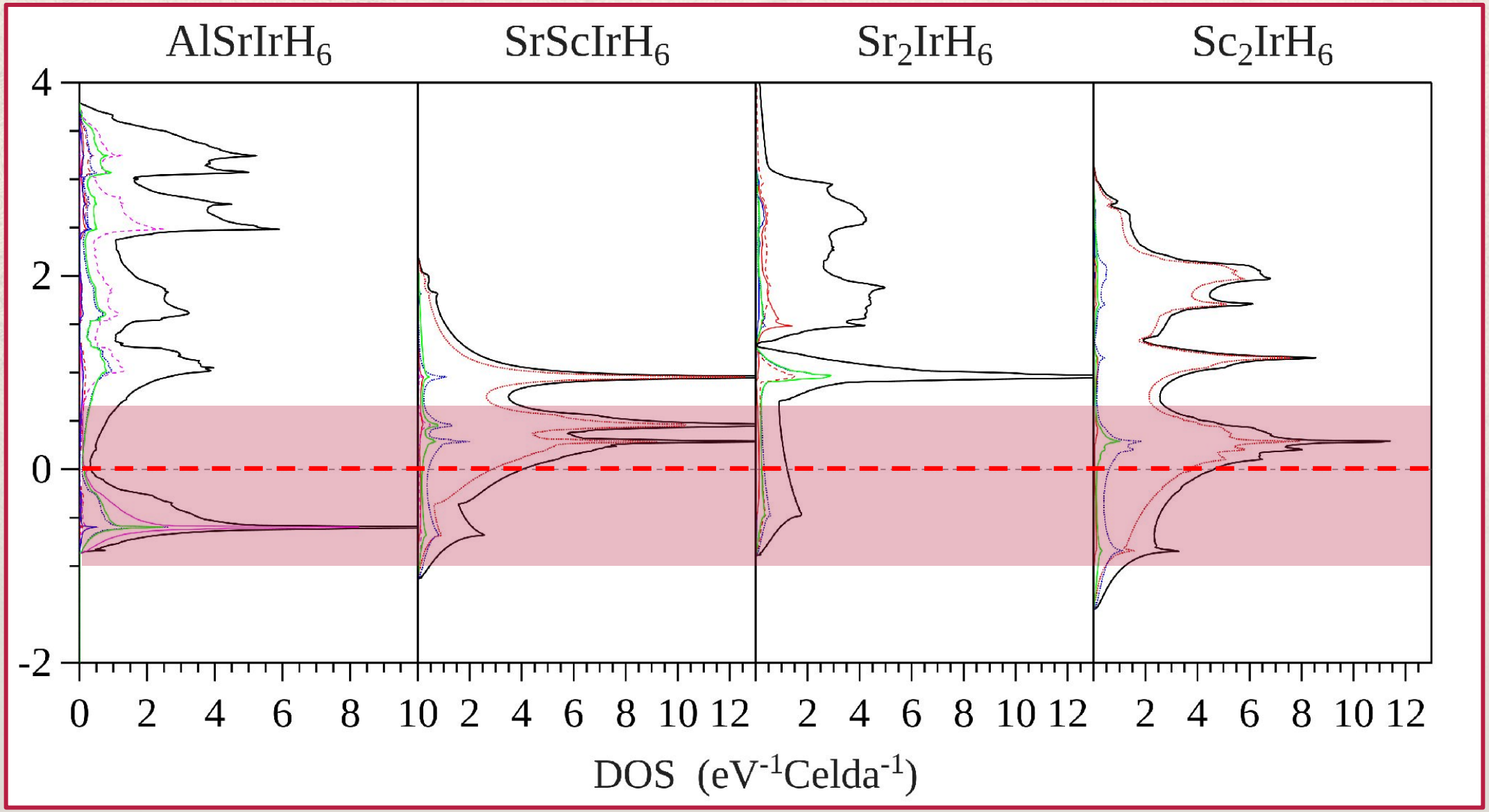




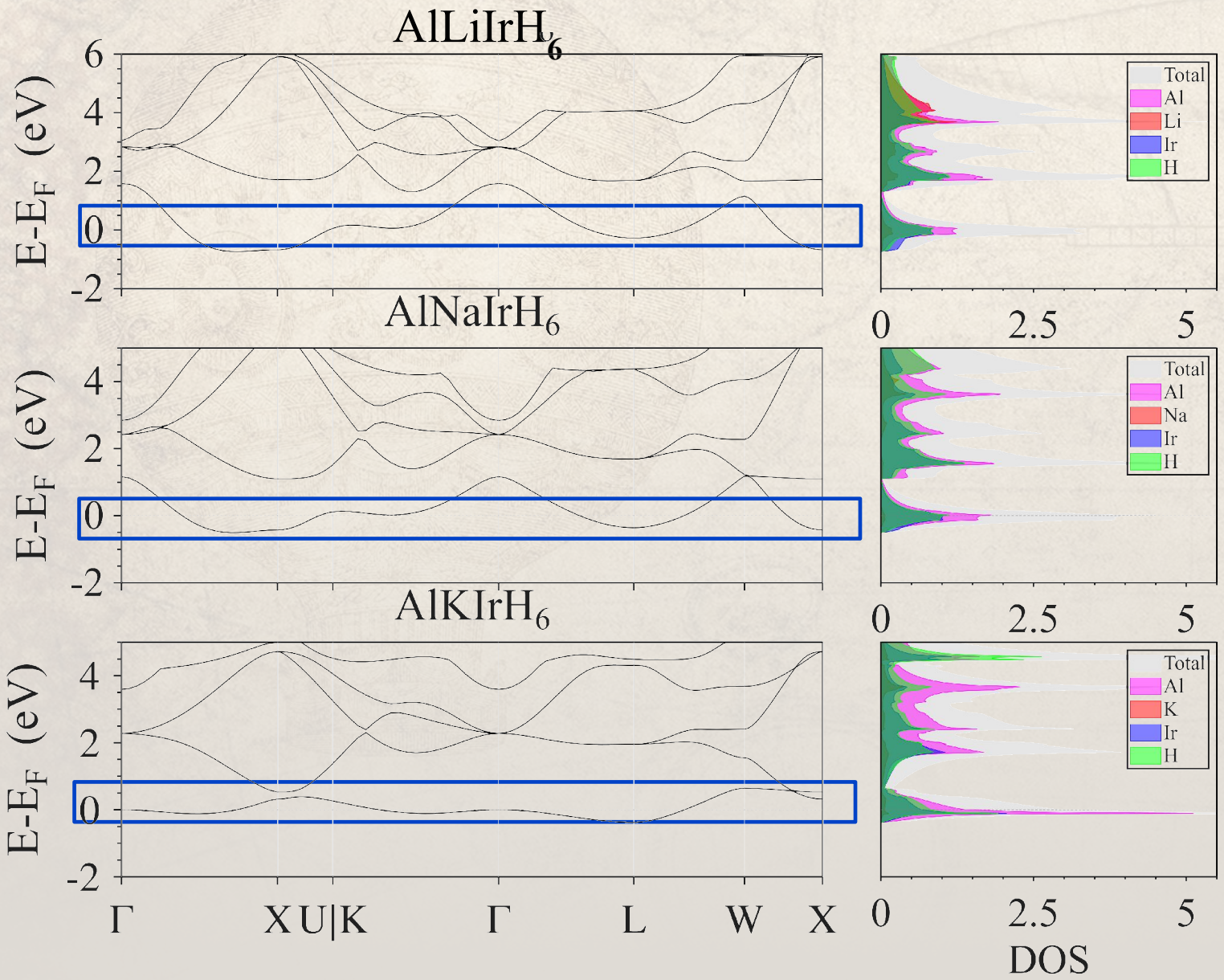


	q (H)	q(Ir)	q(M)
Be_2IrH_6	-0,2455	-1,71	1,593
Mg_2IrH_6	-0,386	-0,987	1,651
Ca_2IrH_6	-0,383	-0,472	1,385
Sr_2IrH_6	-0,399	-0,38	1,387
Ba_2IrH_6	-0,394	-0,269	1,319

AUMENTO DEL NIVEL DE FERMI



BANDAS ULTRAPLANAS: ALUMINO ALCALINOS



	DOS (H)	Ir-H	M-H
$MgIrH_6$	1,1	1,71	2,30
$AlLiIrH_6$	0,75	1,70	2,22
$AlNaIrH_6$	1,15	1,70	2,31
$AlKIrH_6$	0,85	1,68	2,51

	q(H)	q(Ir)	q(M)
$AlLiIrH_6$	-0,302	-1,06	0,87
$AlNaIrH_6$	-0,301	-0,75	0,82
$AlKIrH_6$	-0,273	-0,027	0,71
$AlRbIrH_6$	-0,264	-0,20	0,7

CONCLUSIONS

In terms of the scientific work performed:

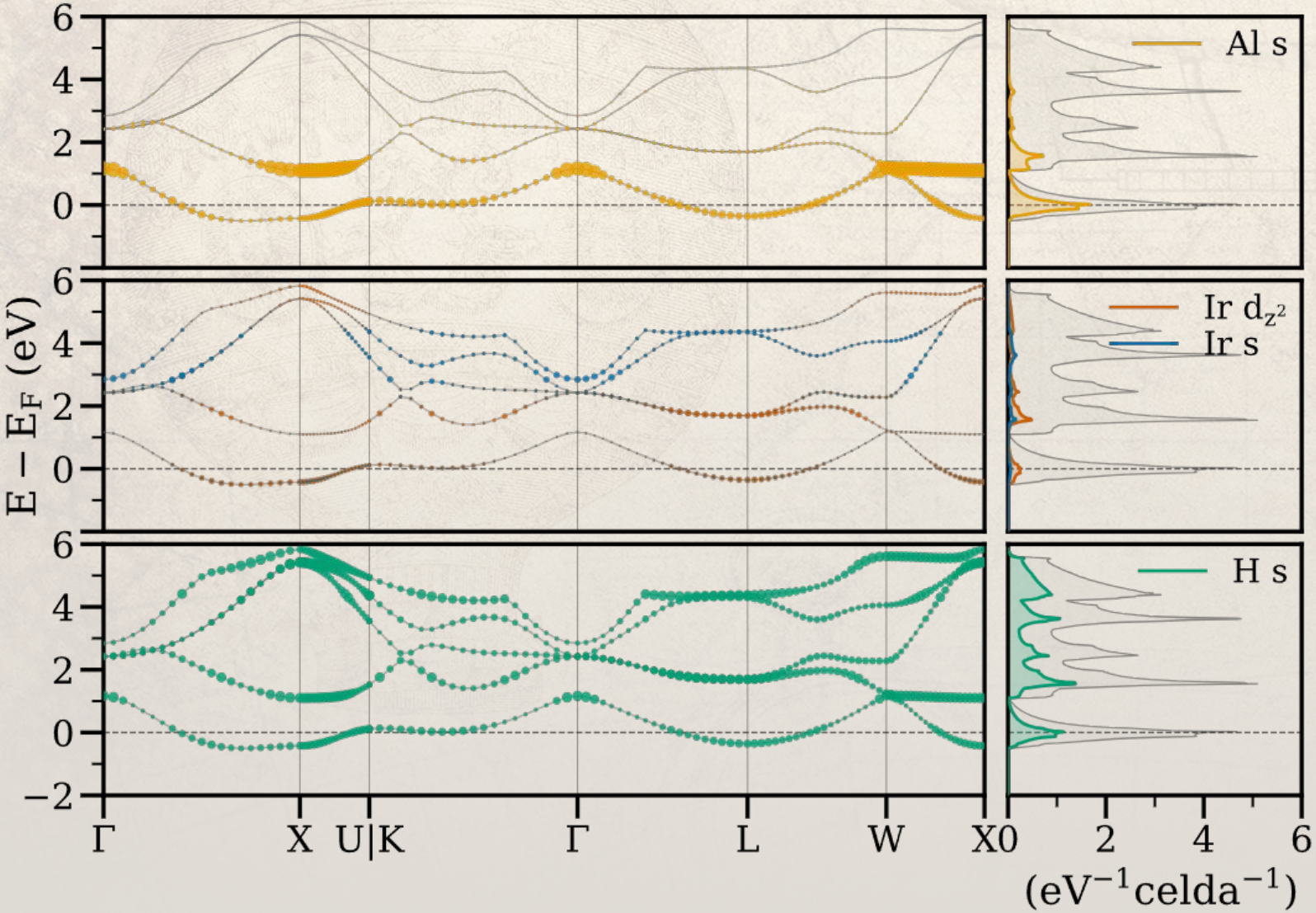
- Comprehension of the Bonding in the family structure of SM_2TMH_6
- Octahedral spacing reduction and the d orbitals needs to be avoided to potentially increase the critical temperature
- Potential Discovery of a New Family of flat band structures.

In terms of learning:

- Knowledge on solid state chemistry and chemical bonding.
- Computational skills
- Understanding of the quantum phenomena

GRACIAS POR SU ATENCIÓN

ESTRUCTURAS ALUMINO-ALCALINAS. BANDAS ULTRAPLANAS

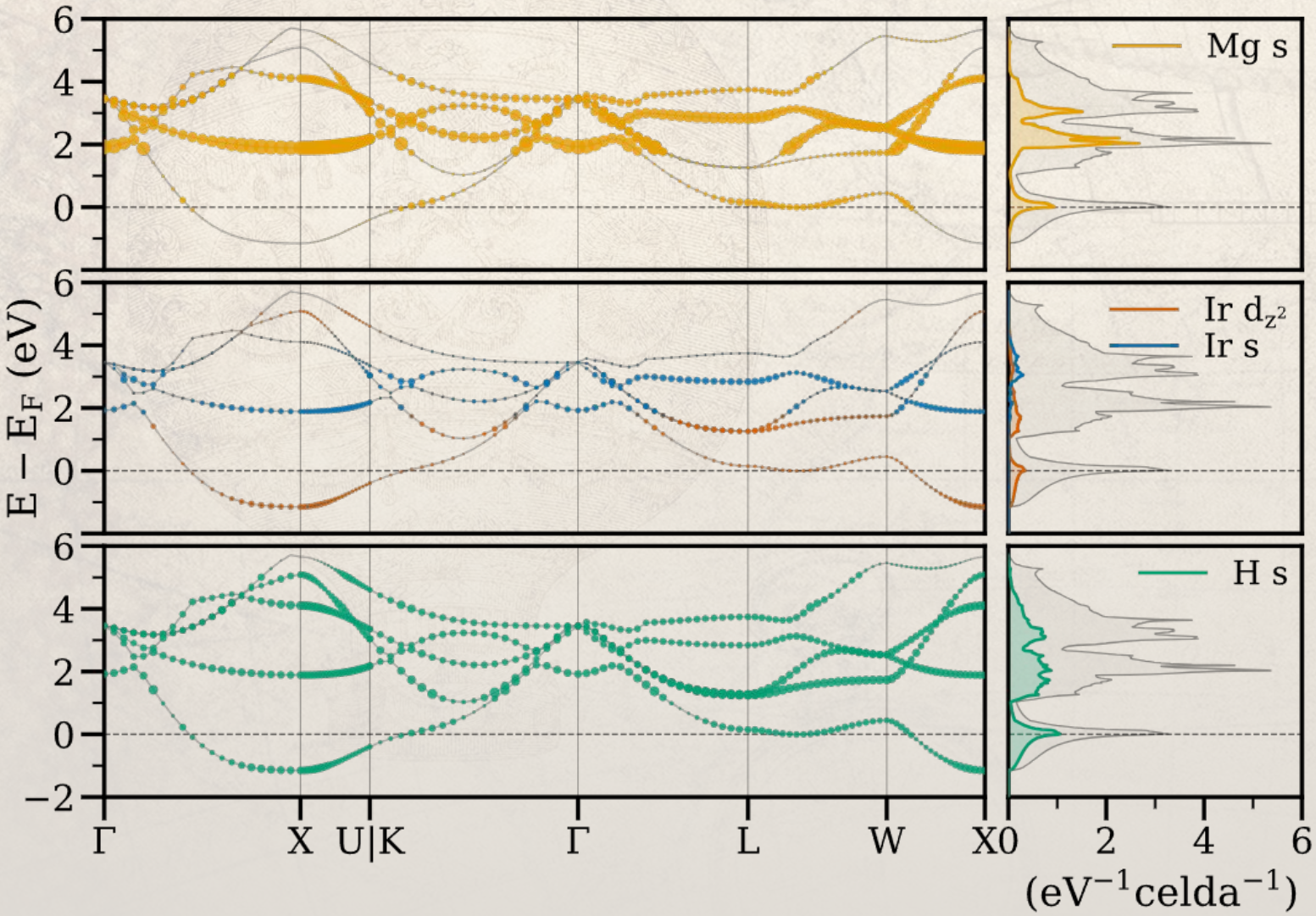


X — Contribuciones de Orbitales 1s(H), dz^2(Ir) y Al(s).

L — Contribuciones de Orbitales 1s(H), dz^2(Ir) y Al(s).

Γ — Contribuciones de Orbitales 1s(H), 5s(Ir) y Al(s).

ESTUDIO DEL Mg_2IrH_6

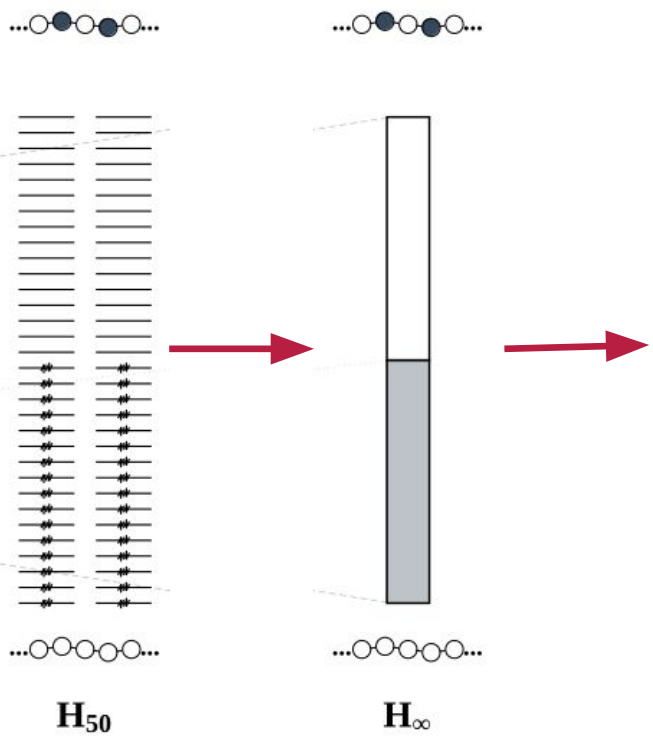


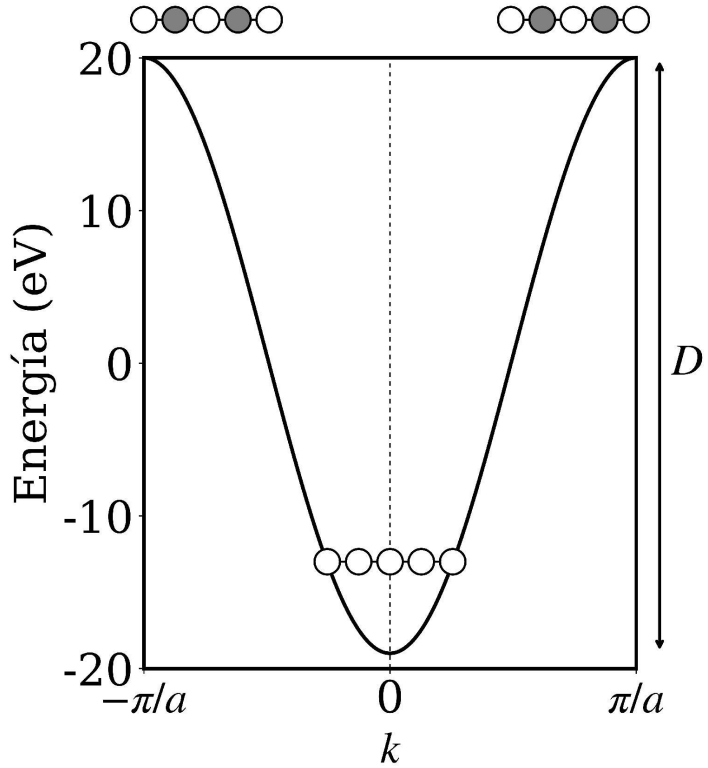
X — Contribuciones de Orbitales 1s(H) y dz^2(Ir)

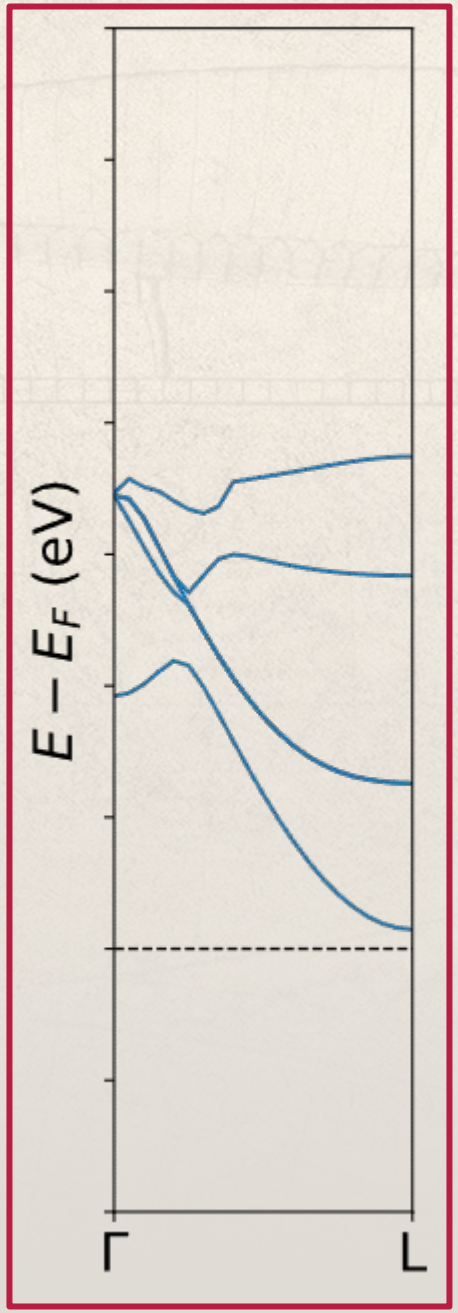
L — Contribuciones de Orbitales 1s(H), dz^2(Ir) y Mg(s).

Γ — Contribuciones de Orbitales 1s(H), 5s(Ir) y Mg(s).

QUÍMICA DE ESTADO SÓLIDO







Γ

L