10th ABINIT International Developer Workshop

Coulomb kernel cut-off methods in ABINIT ground-state calculations

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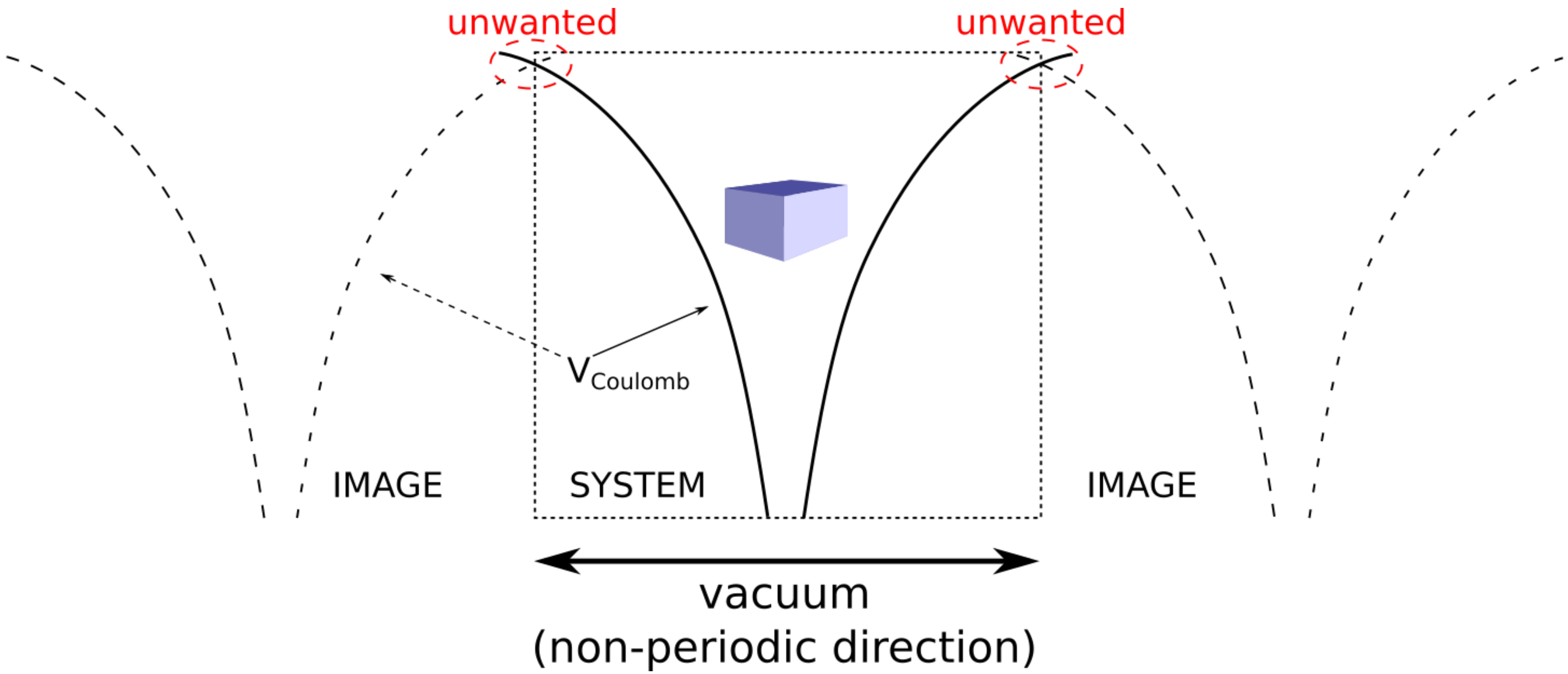
IMCN

What is the problem?



2 solutions in the PW framework

Increase vacuum size
Advantage: Use the code as is
Disatvantage: Computationally costly very fast!

Truncate the Coulomb potential
Advantage: Needs less "vacuum"
Disatvantage: Needs implementation

Where it all started...

- GW suitable methods to treat the Coulomb singularity **G** = 0
- Currently available in ABINIT:

Not necessary in ground-state

- ERFC
- ERF
- Monte-Carlo integration in miniBZ integration
- auxiliary functions for 3D systems

Necessary in ground-state

- Spherical (0D or 3D)
- Cylinder (1D)
- Surface (2D)

- ERFC

Only for HSE XC

Outline

- Coulomb kernel truncation methods
- Changes inside ground-state ABINIT
- Showcases for 2D and 1D scenarios
- Forthcoming work

Truncation of the Coulomb Kernel (I)

$$\frac{1}{G^2} \rightarrow \frac{1}{G^2} K_{cutoff}$$

$$\left(\frac{1}{\vec{r}} \rightarrow \frac{\theta(\vec{r}_c)}{|r|} \right)$$

Method	Kernel cut-off	Radius cut-off
0D or 3D - Spencer-Alavi	$G \neq 0 \rightarrow K_{cutoff} = 1 - \cos(GR_{cut})$ $(v_{sphere} = \frac{\theta(r_c)}{\|r\|})$	Default: $R_{cut} = (\frac{3N_k V}{4\pi})^{1/3}$ or user-defined **rcut**

Method	Kernel cut-off	Radius cut-off
1D - Rozzi	$G_x \neq 0$ & $G_\perp =$ any $\rightarrow K_{cutoff} = 1 + G_\perp R J_1(G_\perp R) K_0(\|G_x\| R) - \|G_x\| R J_0(G_\perp R) K_1(\|G_x\| R)$ $G_x = 0$ & $G_\perp \neq 0$ $\rightarrow K_{cutoff} = -\int_0^R r J_0(G_\perp r) \ln(r) dr G^2$ $(v_{cylindrical} = \frac{\theta(r_{xy})}{\|r\|})$	Default: $R = R_\perp/2$ or user-defined **rcut**
1D - Beigi	$K_{cutoff} \leftarrow \int_0^{h_x} dx \int_0^{h_y} dy \theta(x,y) 2K_0(\|k_z\|R) \cos(k_x x + k_y y)$ $(v_{wire} = \frac{\theta(x,y)}{\|r\|})$	Default: $h_x = R_x/2$ $h_y = R_y/2$ or user-defined **rcut**

Method	Kernel cut-off	Radius cut-off
2D - Rozzi	$G_\parallel \neq 0$ & $G_\perp =$ any $\rightarrow K_{cutoff} = 1 + e^{-G_\parallel R}[G_\perp/G_\parallel sin(G_\perp R) - cos(G_\perp R)]$. $G_\parallel = 0$ & $G_\perp \neq 0$ $\rightarrow K_{cutoff} = 1 - \cos(G_\perp R) - G_\perp R \sin(G_\perp R)$	Default: $R = L_z/2$ or user-defined **rcut**
2D - Beigi	$G \neq 0 \rightarrow K_{cutoff} = 1 - e^{-G_\parallel R} cos(G_\perp R)$ $(v_{sheet} = \frac{\theta(z_c - \|z\|)}{\|r\|})$	Default: $R = L_z/2$ or user-defined **rcut**

*Spencer, Alavi PRB 77 193110 (2008)
*Rozzi et al. PRB 73 205199 (2006)
*Ismail-Beigi PRB 73 233103 (2006)

Truncation of the Coulmb Kernel (II)

$$\frac{1}{G^2} \rightarrow \frac{1}{G^2} K_{cutoff}$$

Hartree potential cut-off

$$4\pi \frac{n(\vec{G})}{G^2} \rightarrow 4\pi \frac{n(\vec{G})}{G^2} K_{cutoff}$$

Ionic potential cut-off

$$-\frac{Z}{V_{BvK}} \frac{4\pi}{G^2} \rightarrow -\frac{Z}{V_{BvK}} \frac{4\pi}{G^2} K_{cutoff}$$

Ewald summation

$$\frac{1}{2} \sum_{k,k'} Z_k Z_{k'} \left[\sum_{G\neq 0} \frac{4\pi}{\Omega_0 G^2} e^{i\vec{G}(\vec{\tau}-\vec{\tau_{k'}})} e^{-\frac{G^2}{4\Lambda^2}} \right] \rightarrow \frac{1}{2} \sum_{k,k'} Z_k Z_{k'} \left[\sum_{G\neq 0} \frac{4\pi}{\Omega_0 G^2} e^{i\vec{G}(\vec{\tau}-\vec{\tau_{k'}})} (e^{-\frac{G^2}{4\Lambda^2}} + K_{cutoff} - 1) \right]$$

*valid for 2D methods

Bulk - PRB 55 10355 (1997)

What changed in variables?

Previously:

icutcoul variable

(only available in GW)

Currently:

Ground state: icutcoul

Fock operator: fock_icutcoul

GW : gw_icutcoul

Tests added for icutcoul!(v9/t90)

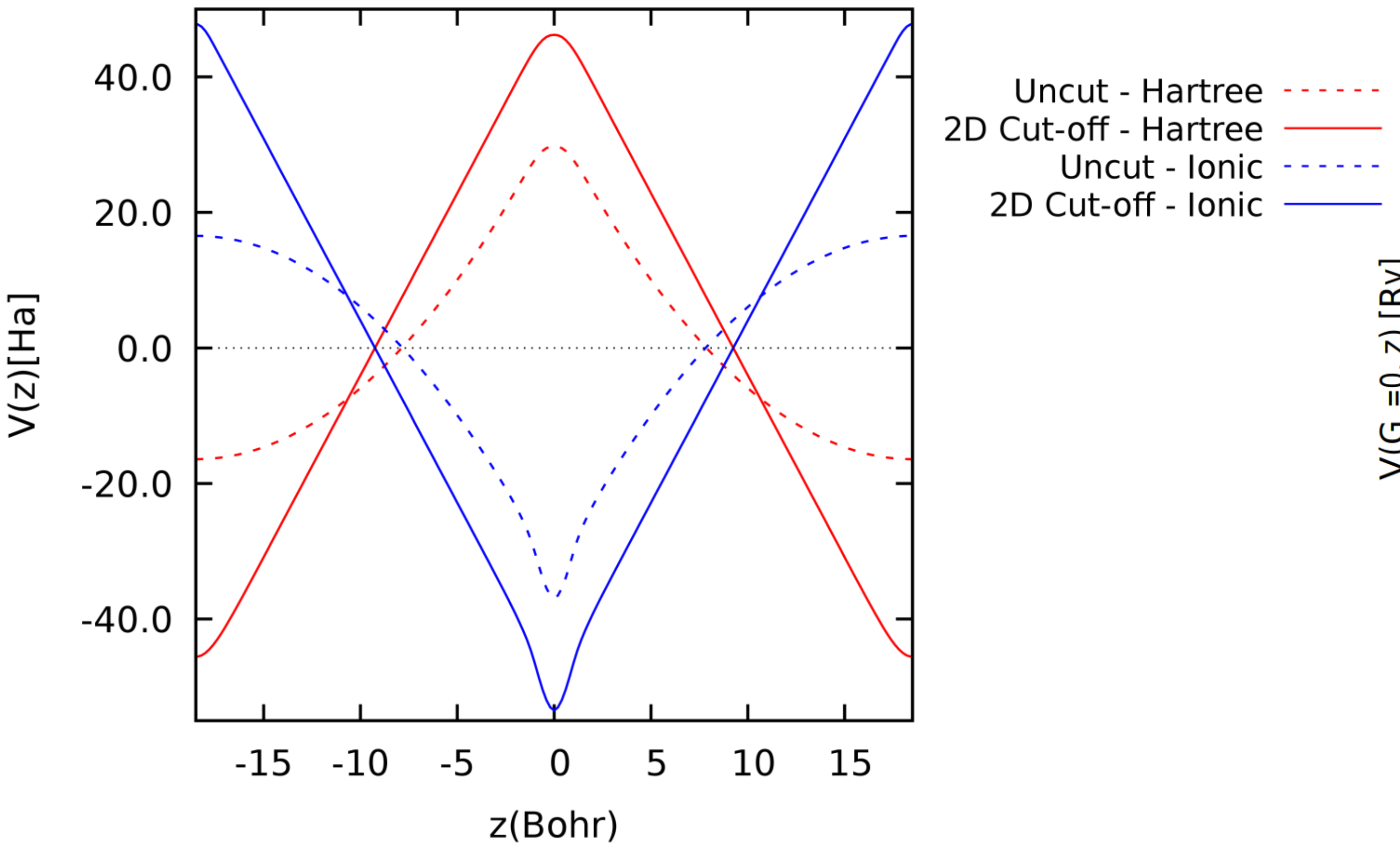
What changed inside the code?

Currently:

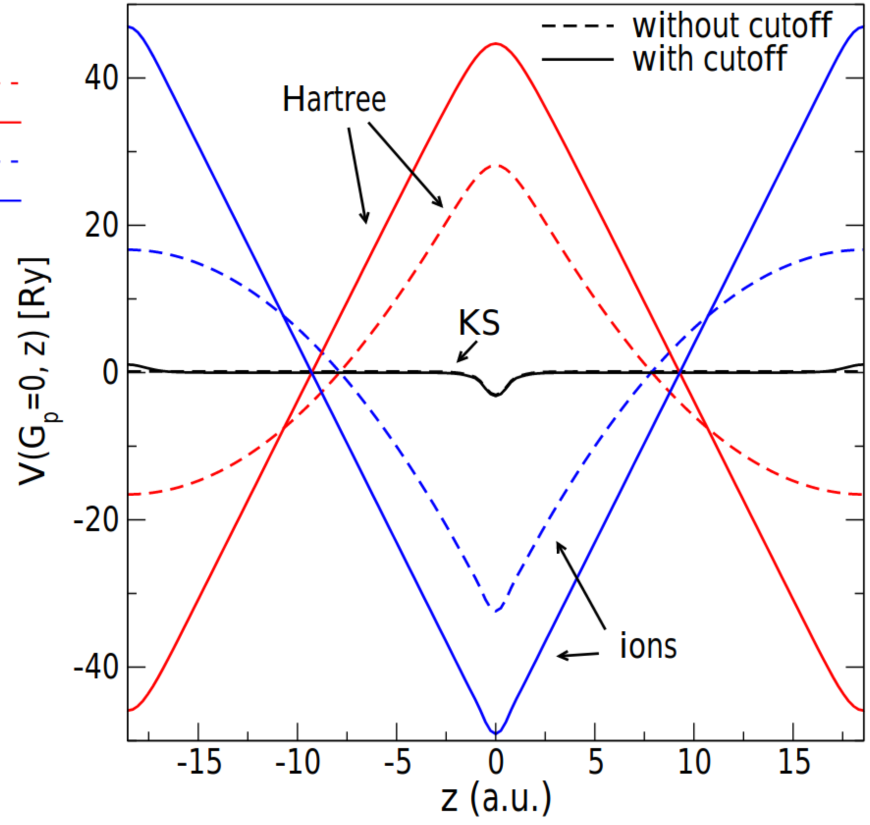
- Modularize vcoul module (GW)
- Transfer and transform the suitable methods in GS
- Created the low level gtermcutoff containing only the K_{cutoff}

Case study – 2D system – Graphene (I)

ABINIT



QuantumEspresso

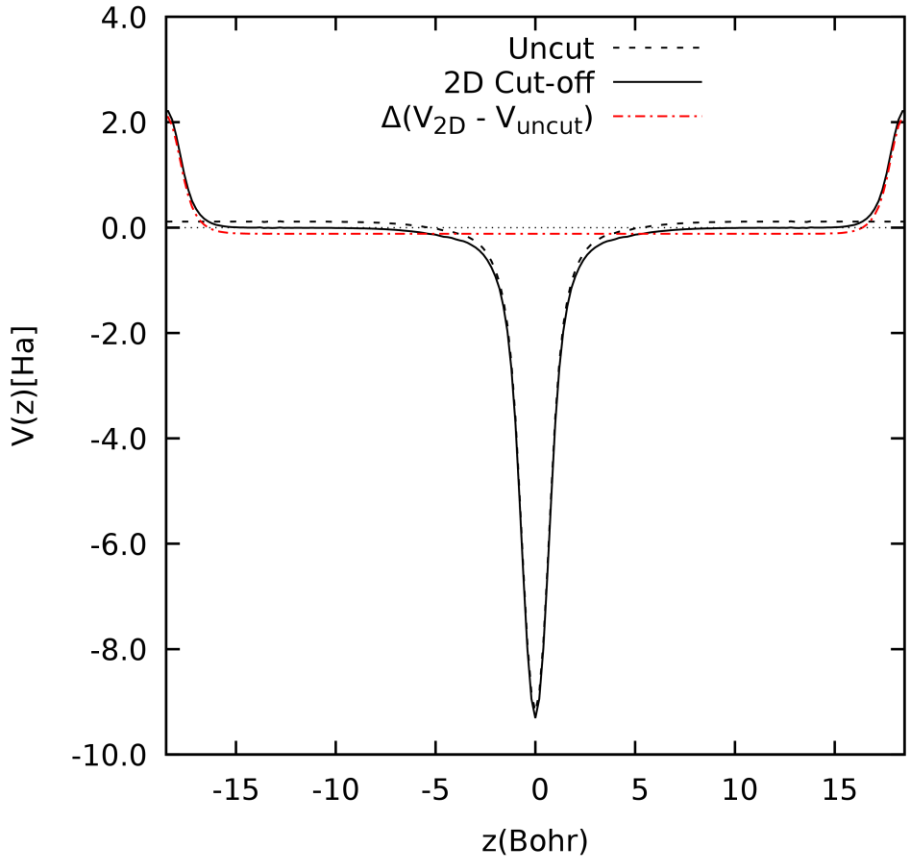


ABINIT: Hartree and Pseudo-potentials of graphene in the untrucated and 2D truncated (Beigi/Rozzi) scenarios

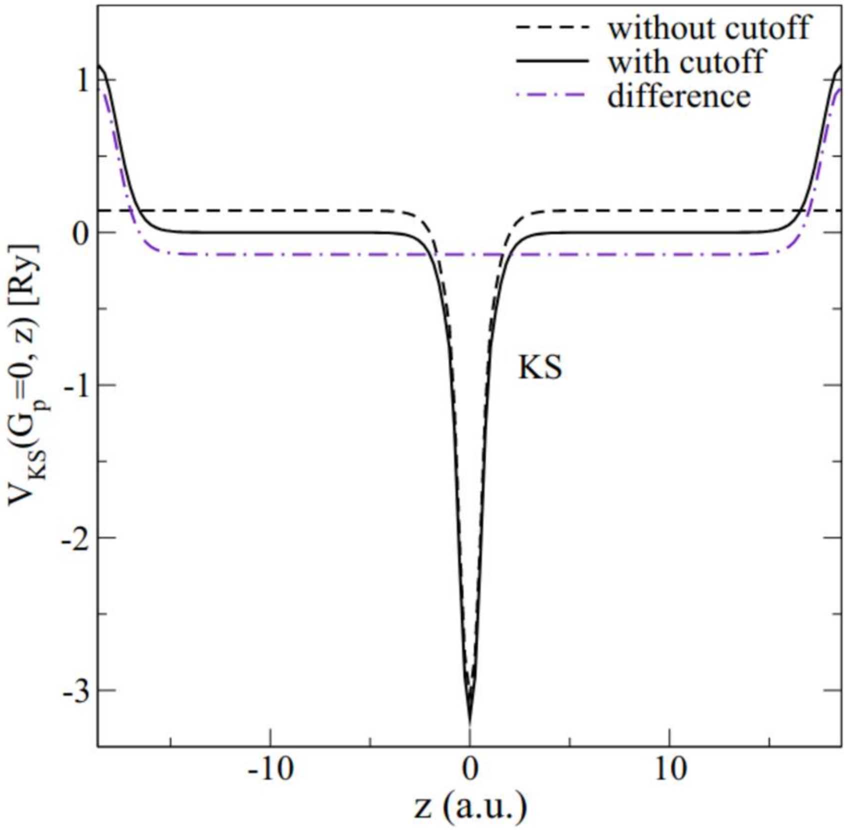
QE: Hartree and Pseudo-potentials of graphene in the untruncated and truncated scenarios (PRB 91 165248 2015)

Case study – 2D system – Graphene (II)

ABINIT



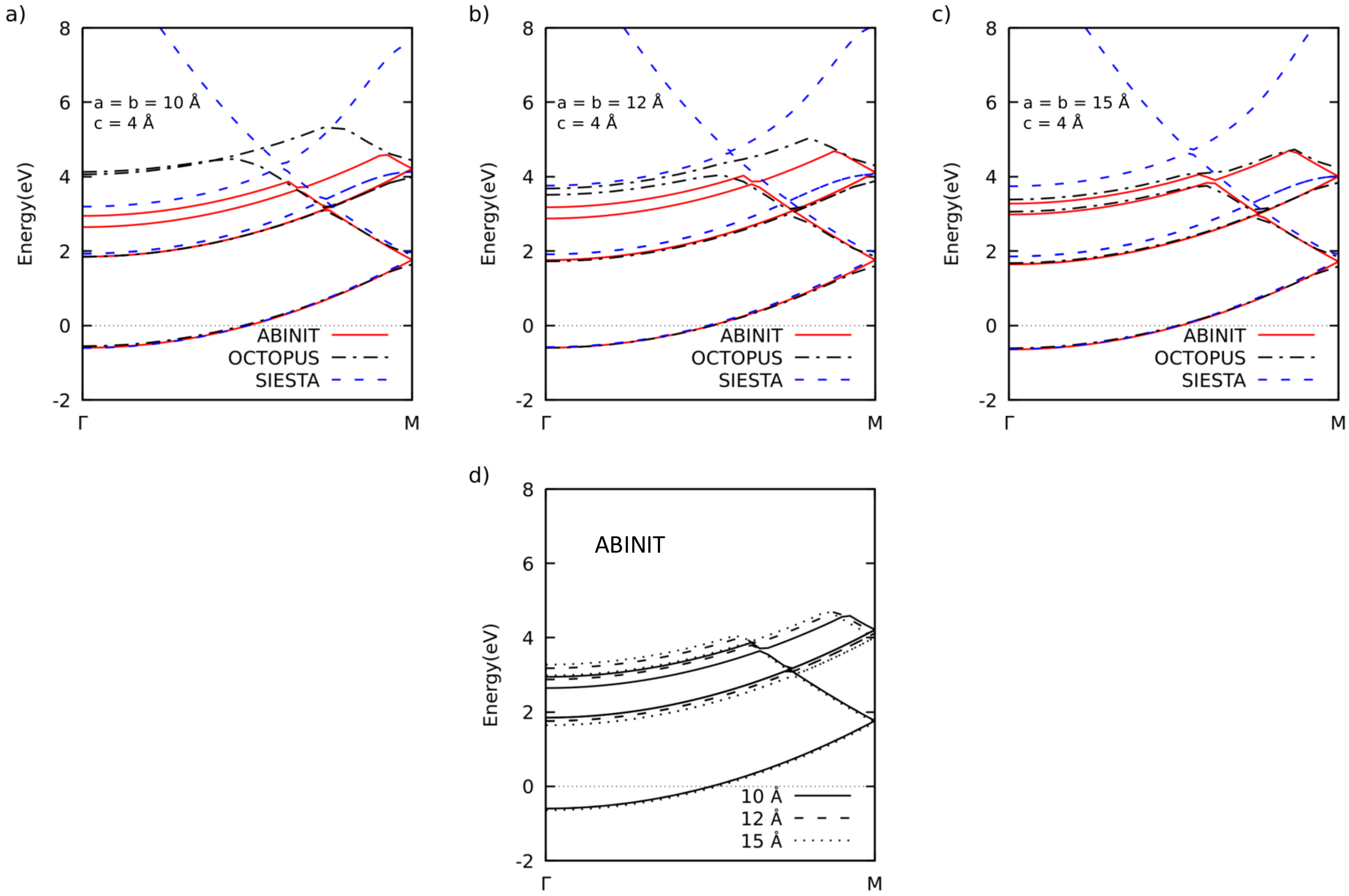
QuantumEspresso



ABINIT: Kohn-Sham potential of graphene in the untrucated and 2D truncated scenarios (Beigi/Rozzi) obtained in ABINIT

QE: Kohn-Sham potential of graphene in the untruncated and truncated scenarios obtained in QE (PRB 91 165248 2015)

Case study – 1D systems – Na chain



Forthcoming work

Ground state formalism applied to:

- Ewald summation implementation for 2D, 1D and 0D
- Forces and stresses implementation
- DFPT (Hopefully!)

Case study – 2D system – Graphene (III)

	CENTER (Ha)	EDGE (Ha)
Pseudo-Dojo – LDA	-4.641987	1.103180
ABINIT - ONCVPSP	-3.275693	0.897288
LDA – HGH	-14.462906	1.723148
LDA – TM	-6.733732	1.484205
LDA – GTH	-14.587011	1.725340
LDA – FHI	-4.316949	1.236310
LDA – Extra core	-9.837990	1.883866
GGA – FHI	-3.767340	1.223365
CP2K – Goedecker	-15.176940	1.718365
GGA – HGH	-14.433046	1.705526
GGA – Opium	8.421542	0.242951
GGA – HCTH407	-15.429629	1.699490
GGA – HCTH120	-15.565880	1.706209