ADHESIVE FORCES ON HELIUM IN NONTRIVIAL GEOMETRIES

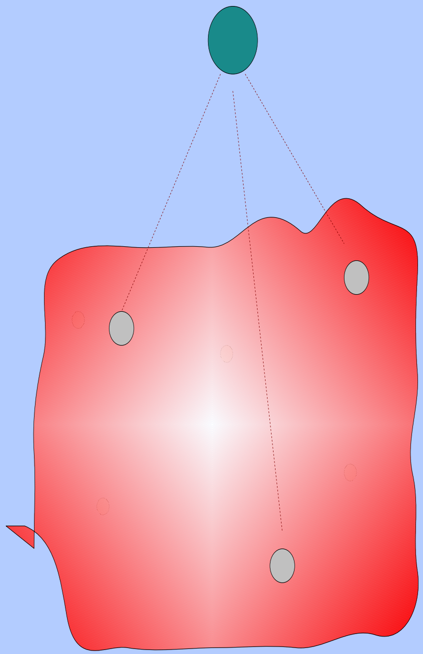
E. S. H.[1]*, A. Hernando*[2]*, R. Mayol*[2] *and M. Pi*[2]

shernand@df.uba.ar

[1]*University of Buenos Aires, Argentina*

[2]*University of Barcelona, Spain*

Vapor particle + matter



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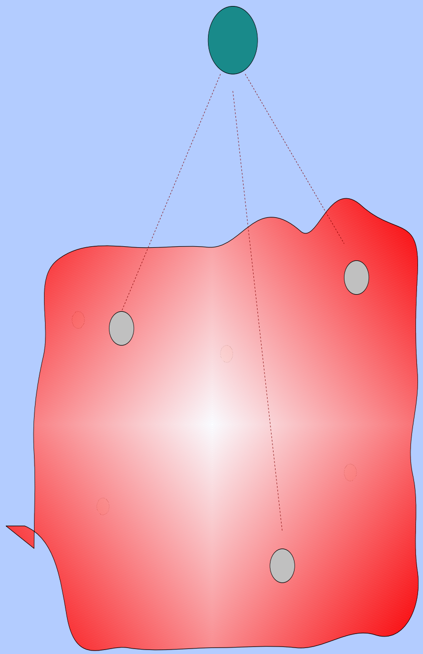

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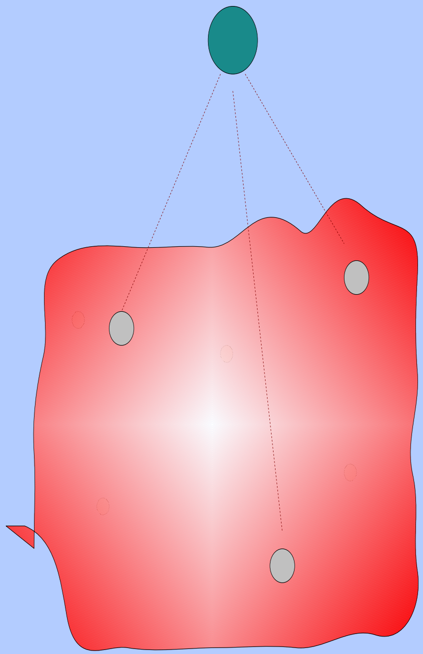

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$$U(\mathbf{r}) = \int d\mathbf{r}'\, n(\mathbf{r}')\, V(\mathbf{r} - \mathbf{r}')$$

A popular choice

$$\boxed{V_{LJ}(\mathbf{r}) \equiv V_{6-12}(\mathbf{r}) = \varepsilon \, \left[\left(\frac{r_{min}}{r}\right)^{12} - 2 \, \left(\frac{r_{min}}{r}\right)^{6} \right]}$$

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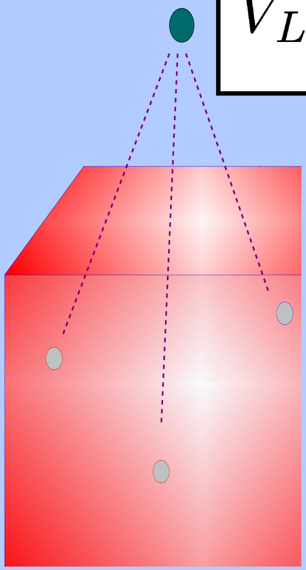

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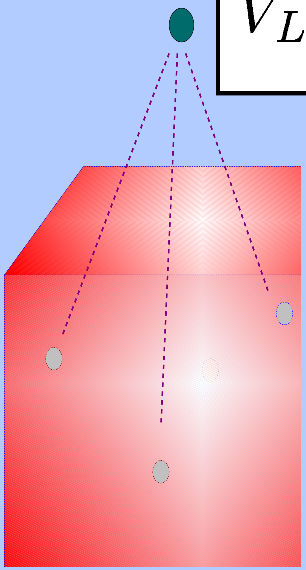

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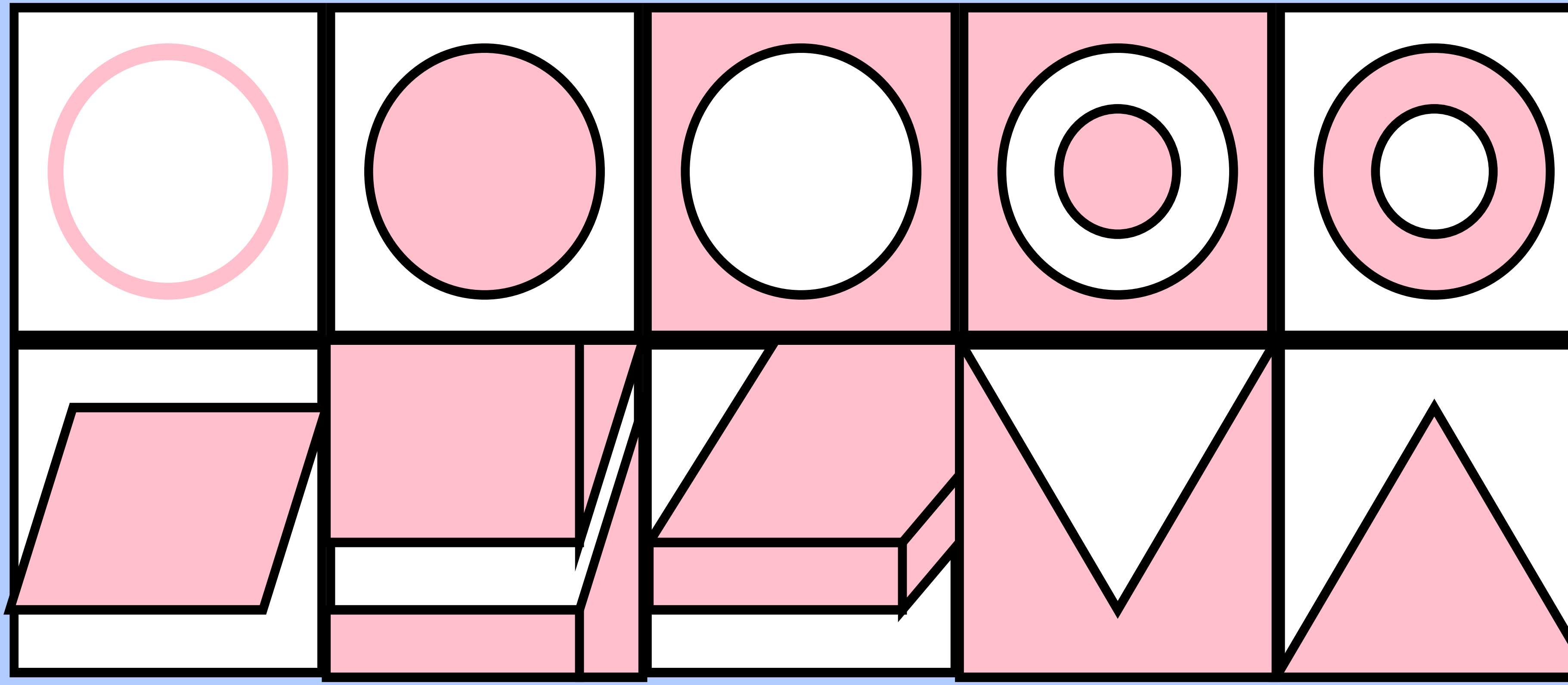
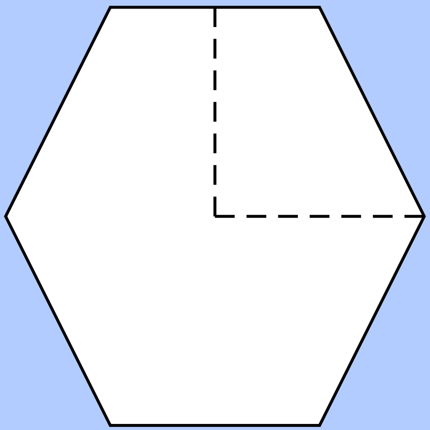
$$U(z) \equiv V_{3-9}(z) = \frac{D}{2} \left[\left(\frac{z_{min}}{z}\right)^{9} - 3 \left(\frac{z_{min}}{z}\right)^{3} \right]$$

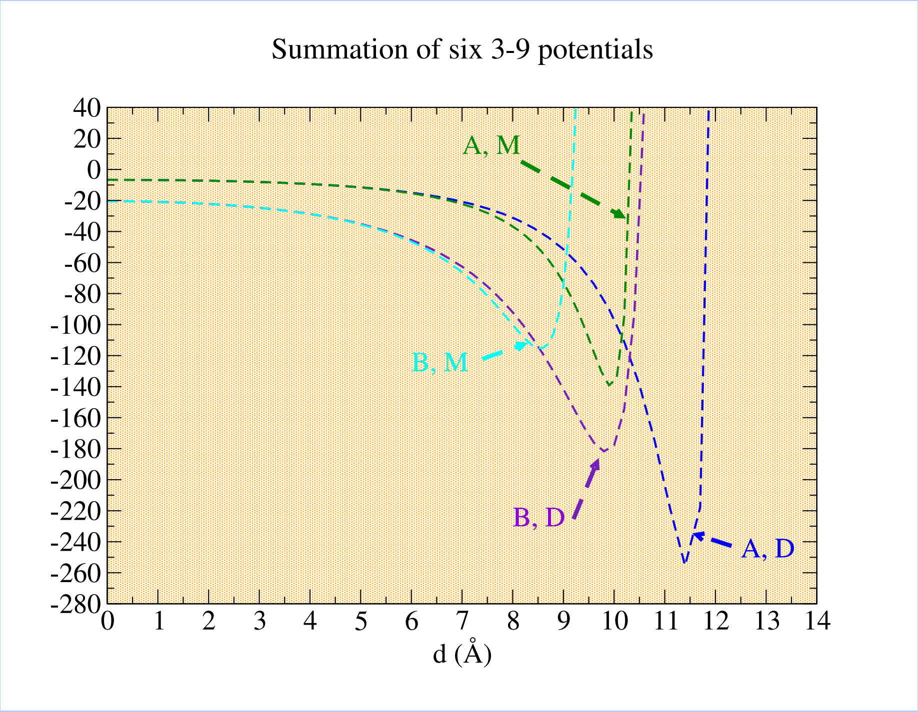
Geometries with high symmetry

The LJ potential is analytically integrable (or quasiintegrable)



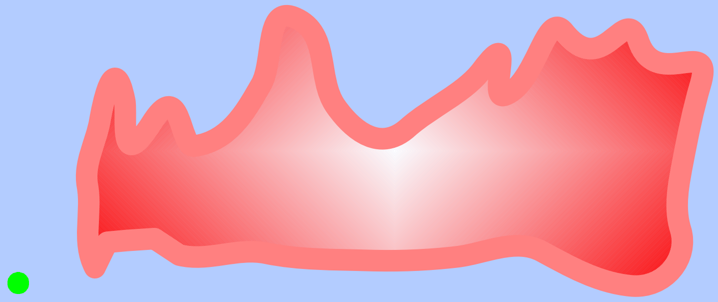
FSM-16 hexagonal pores with six 3-9's





(from M. Rossi, D. E. Galli and L. Reatto, JLTP **146**, 98 (2006))

Open questions



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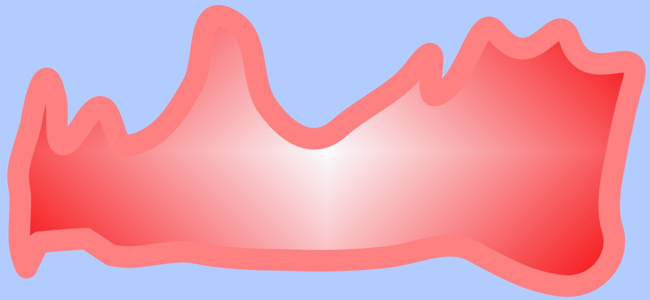

- How legitimate is the continuum hypothesis?

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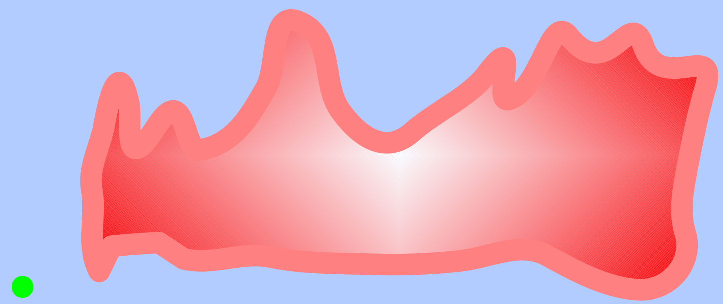

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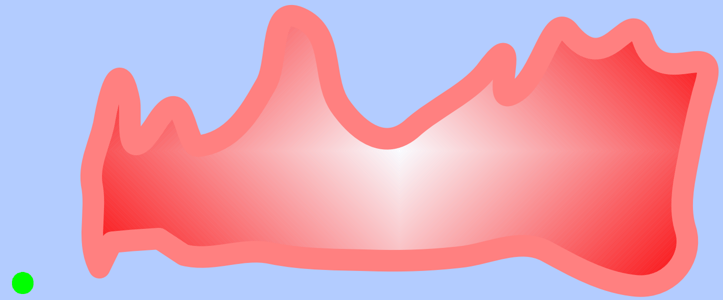

- How legitimate is the continuum hypothesis?
- How accurate is a LJ potential?
- For metallic planar half-solids, an *ab-initio* $U(z)$ is

$$\boxed{U_{CCZ}(z) \neq \int d\mathbf{r}' \, n(\mathbf{r}') \, V_{pair}(\mathbf{r} - \mathbf{r}')}$$

(A. Chizmeshya, M. W. Cole, and E. Zaremba, J. Low Temp. Phys. 110, 677 (1998).)

New question

Is the inverse problem solvable?, *i.e.*, given $U_{ref}(z)$, can we find sources $V(\mathbf{r}-\mathbf{r}')$?

$$U_{ref}(z) = \int_{-\infty}^{0} dz' \int\int dx'dy'\, V(\mathbf{r}-\mathbf{r}')$$

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$$U_{ref}(z) = \int_{-\infty}^{0} dz' \int\int dx'dy'\, V(\mathbf{r}-\mathbf{r}')$$

If so, then for *almost any* geometry,

$$U(\mathbf{r}) = \int d\mathbf{r}'\, n(\mathbf{r}')\, V(\mathbf{r}-\mathbf{r}')$$

It is solvable!

For a half-solid with bulk density ρ_0,

$$\boxed{V(z) = \frac{U''_{ref}(z)}{2\pi\rho_0 z}}$$

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true for the LJ family

$$V_{6-12}(r) = \frac{V''_{3-9}(r)}{2\pi\rho_0 r}$$

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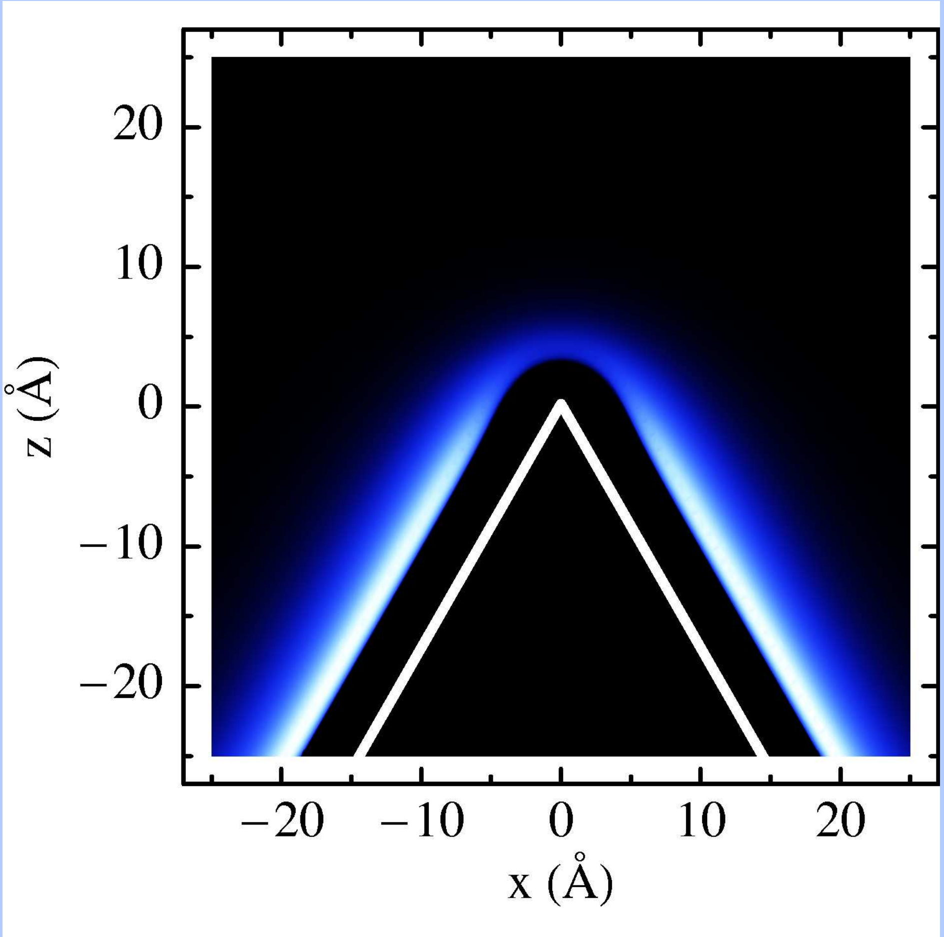
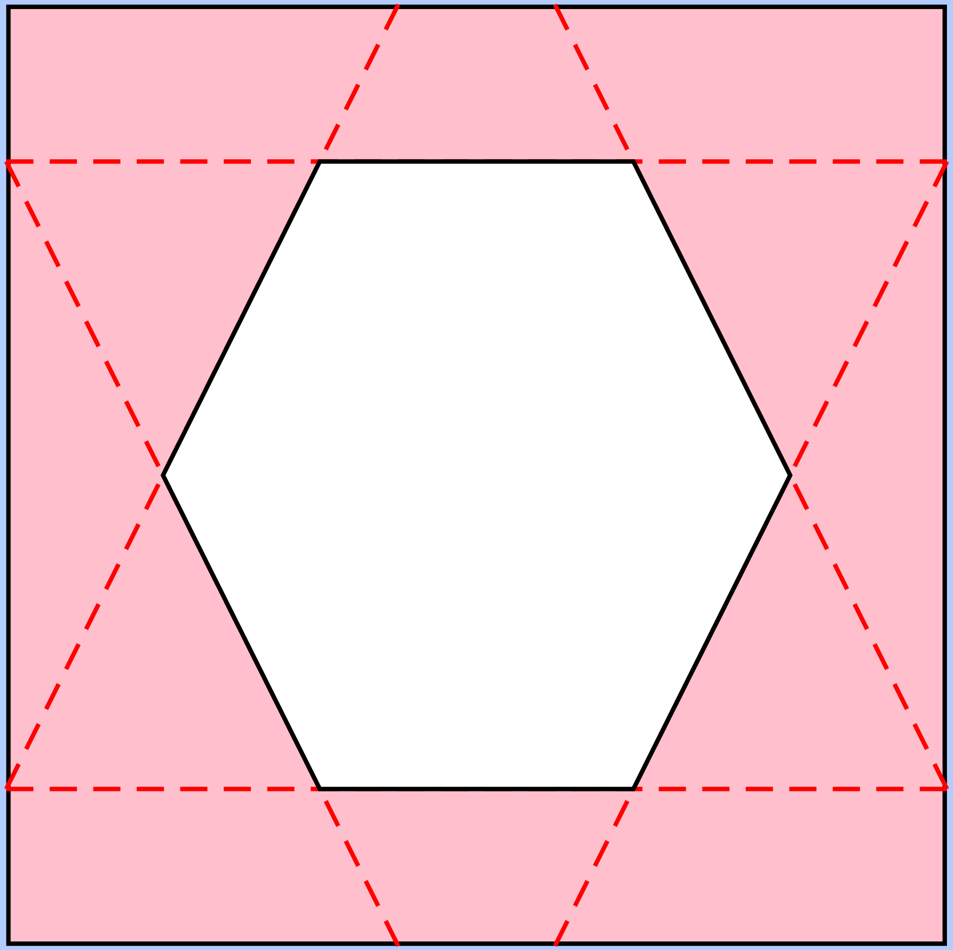
so that for other matter distributions $n(\mathbf{r}')$

$$U(\mathbf{r}) = \int d\mathbf{r}'\, n(\mathbf{r}')\, \frac{U''_{ref}(|\mathbf{r}-\mathbf{r}'|)}{2\pi\rho_0|\mathbf{r}-\mathbf{r}'|}$$

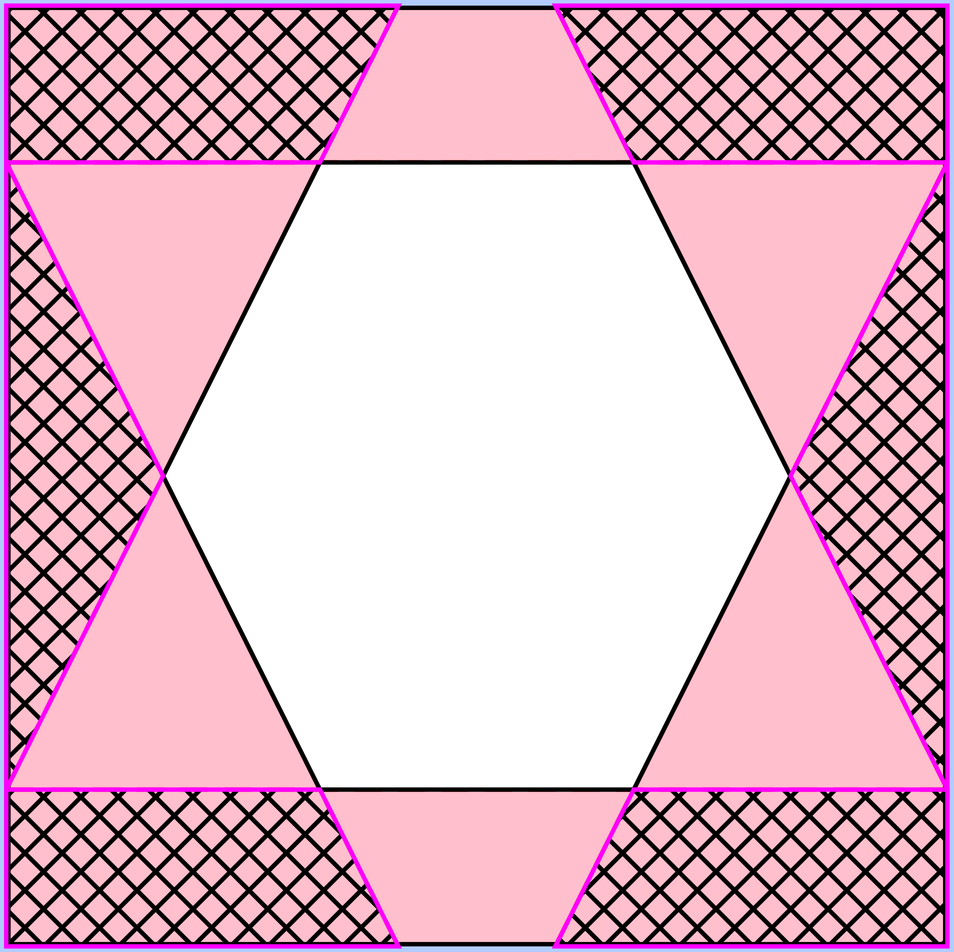
A friendly unit cell



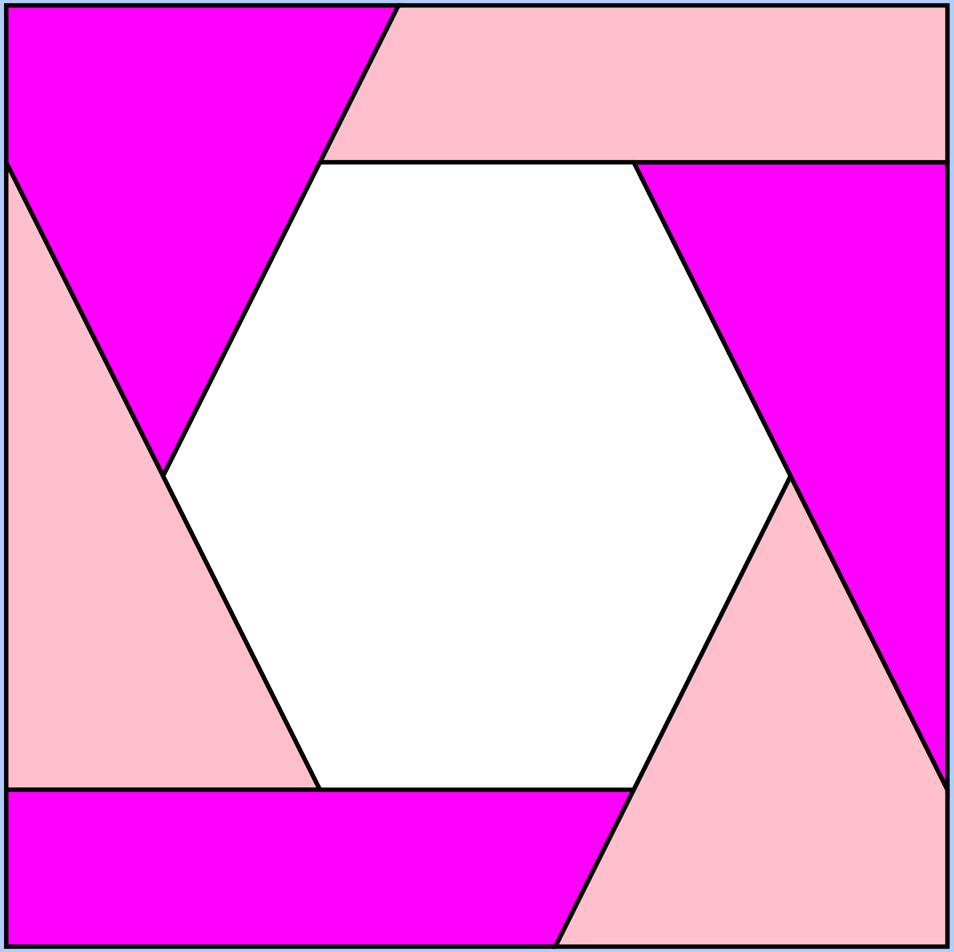
Six half-solids make an hexagonal pore



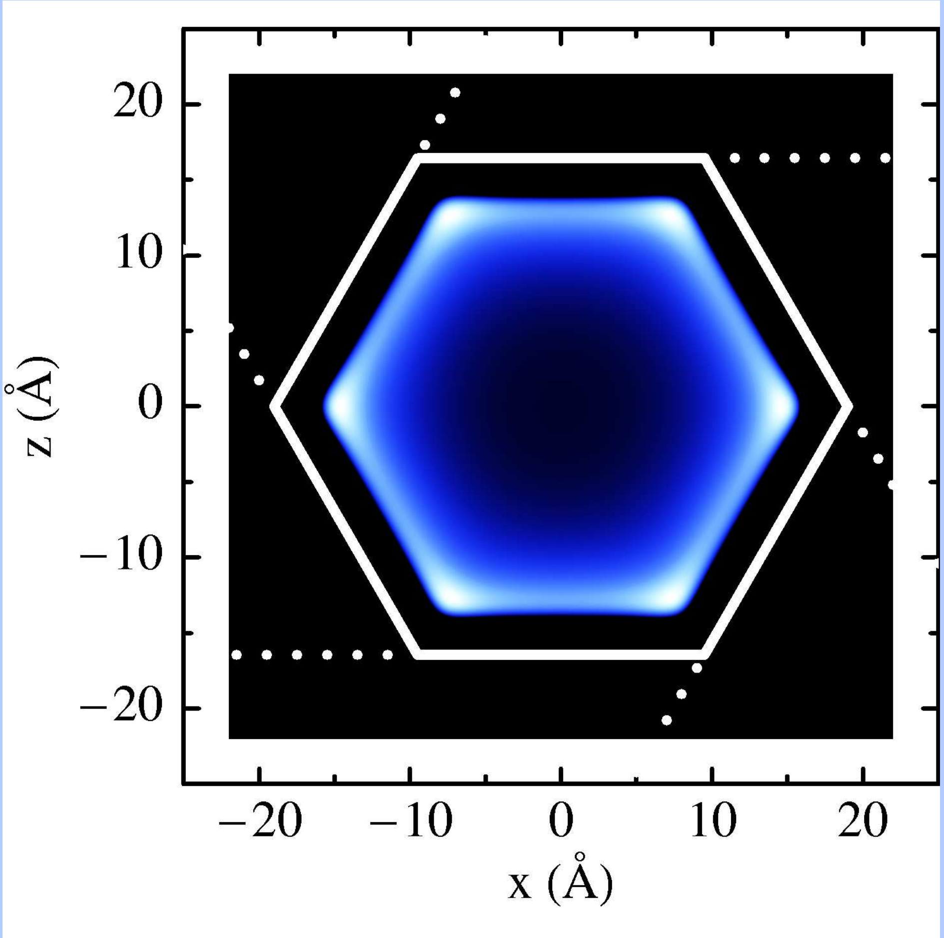
with strong overlap at the vertices



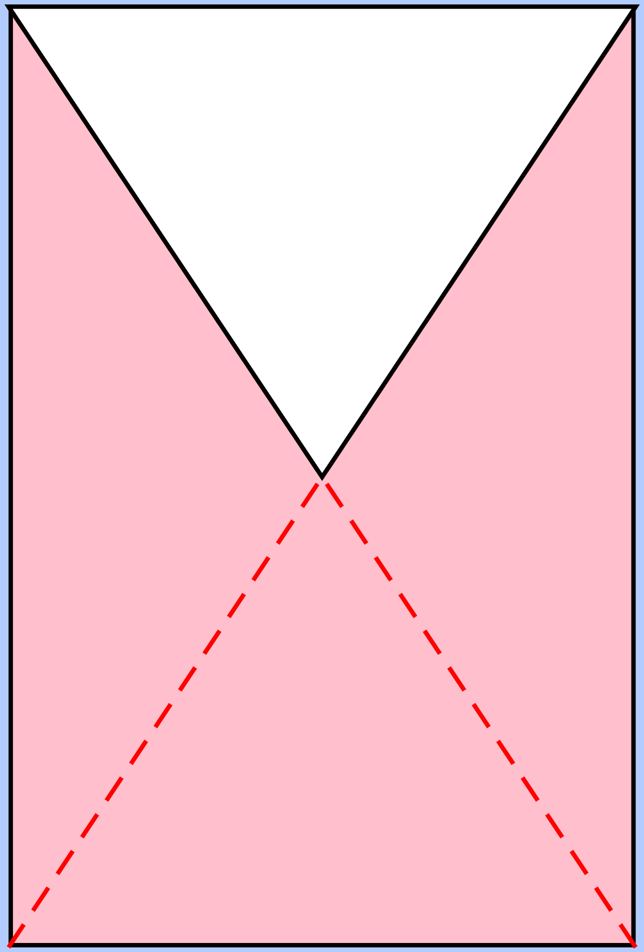
so, we recommend SIX CUSPS INSTEAD



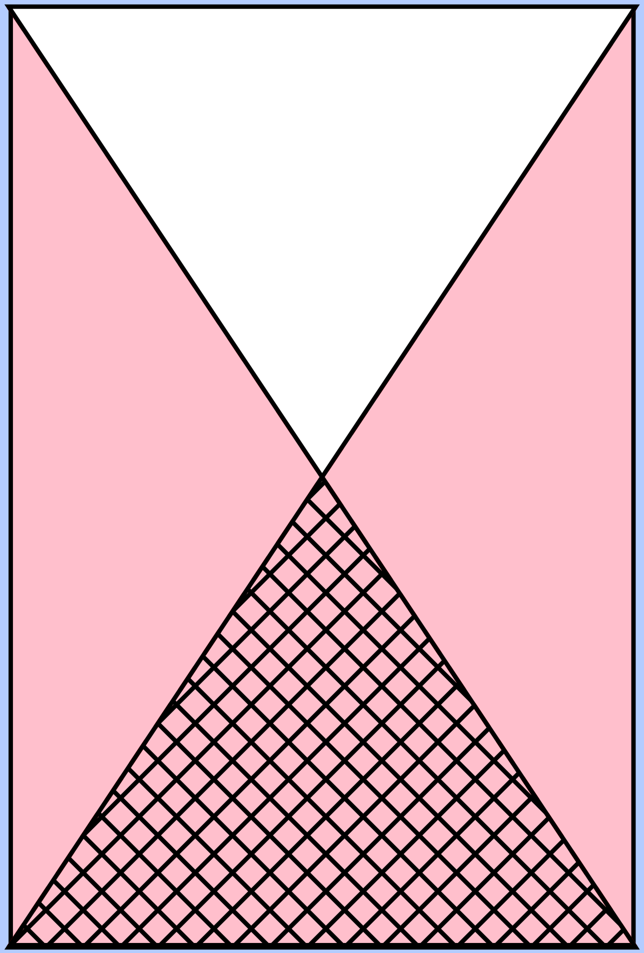
with potential landscape



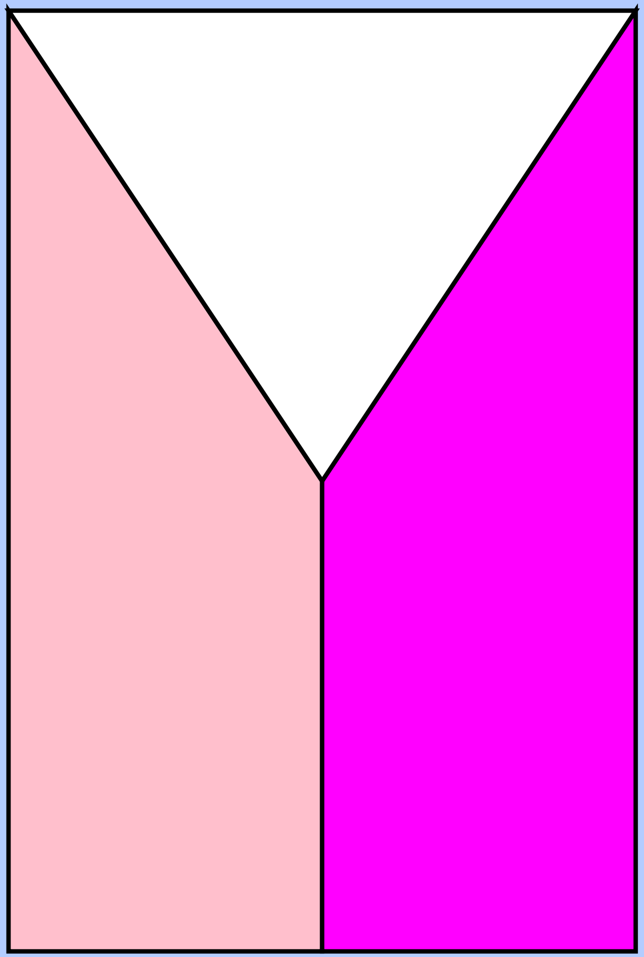
The wedge



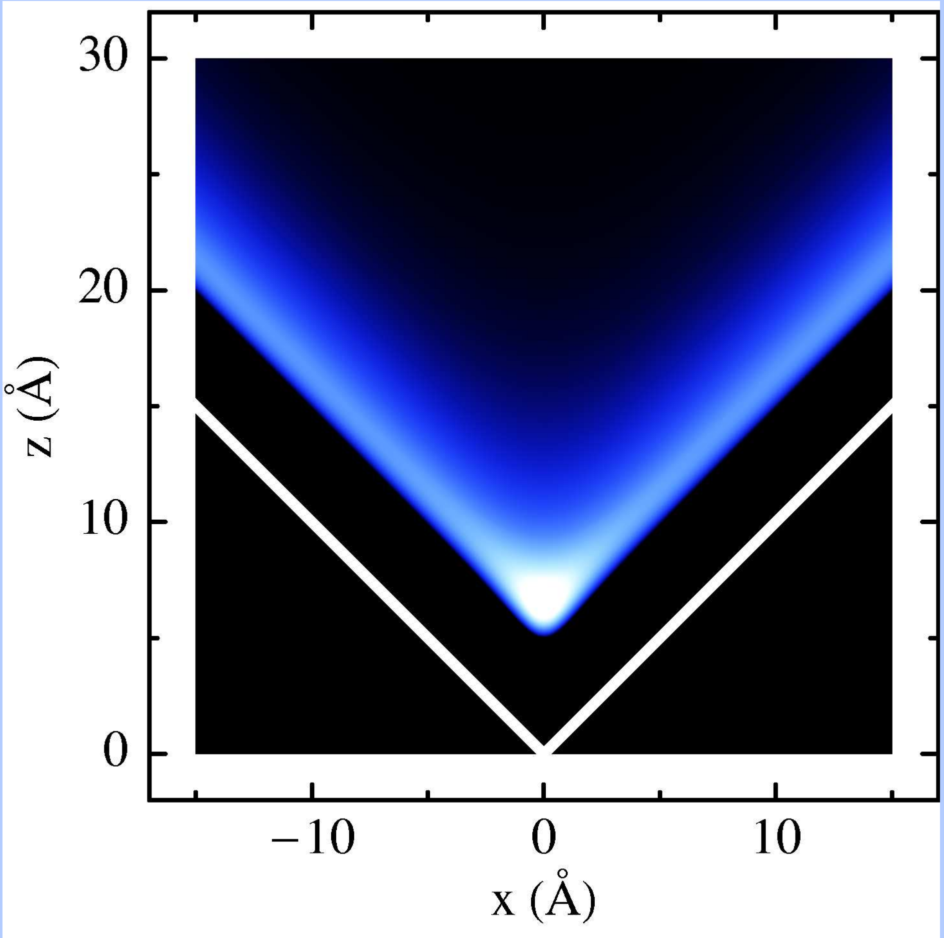
The wedge *was* (ESH *et al* in PRB 73, 245406 (2006))



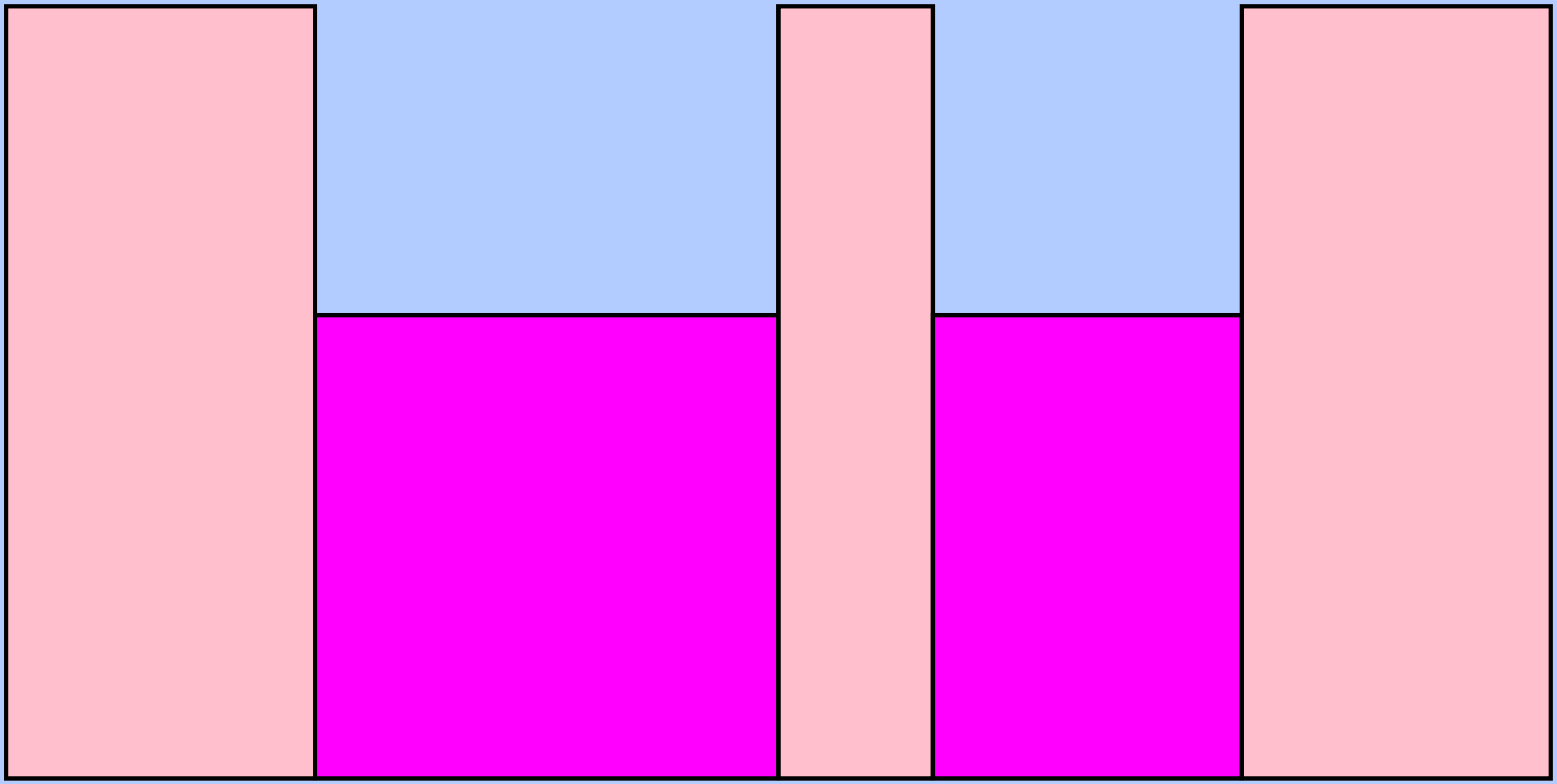
while it may be



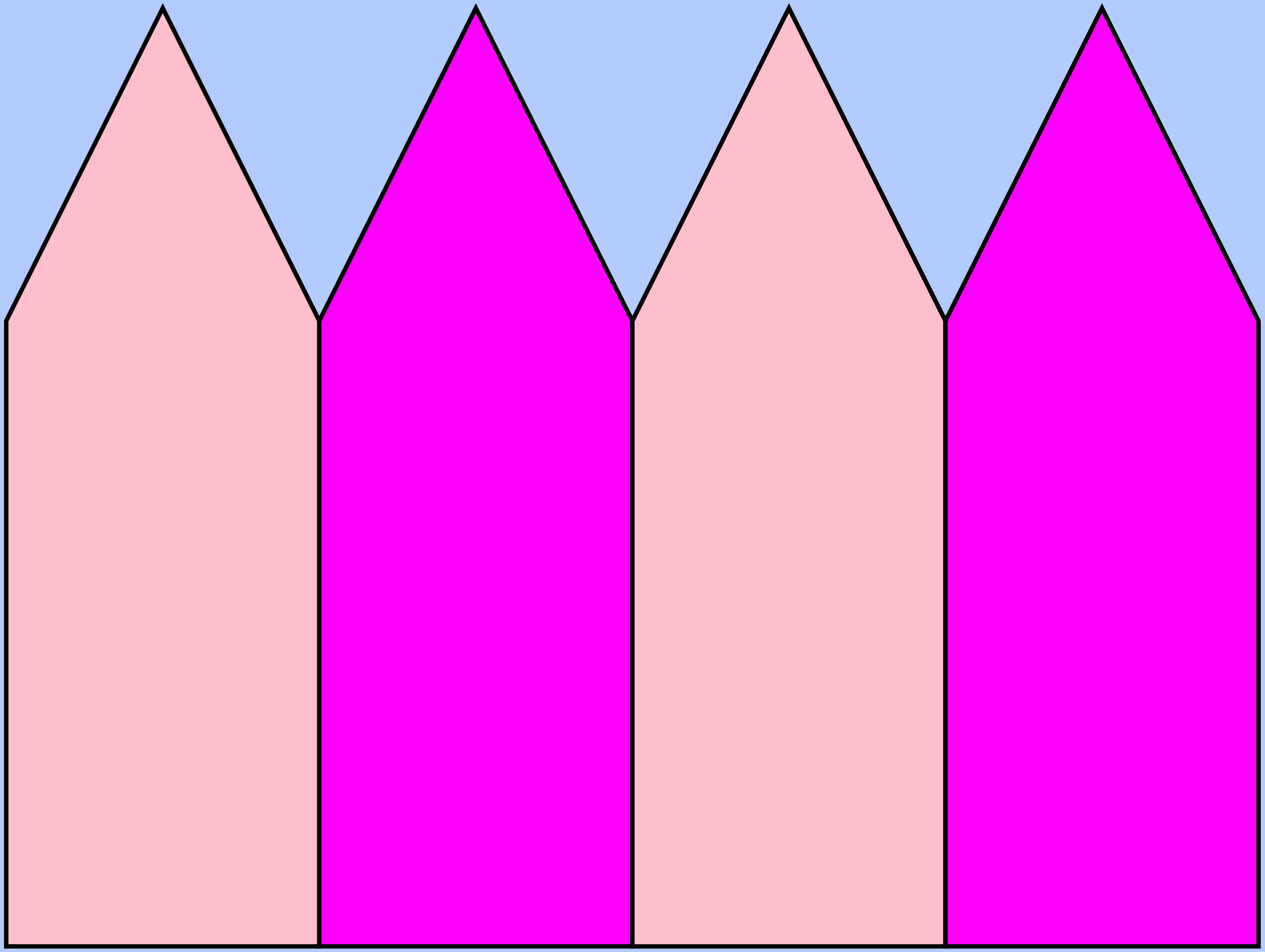
with potential



A striped substrate



A sawtooth substrate



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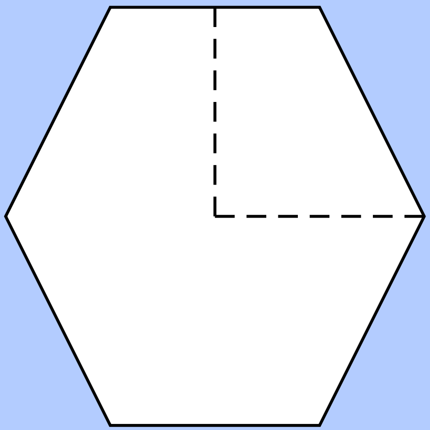

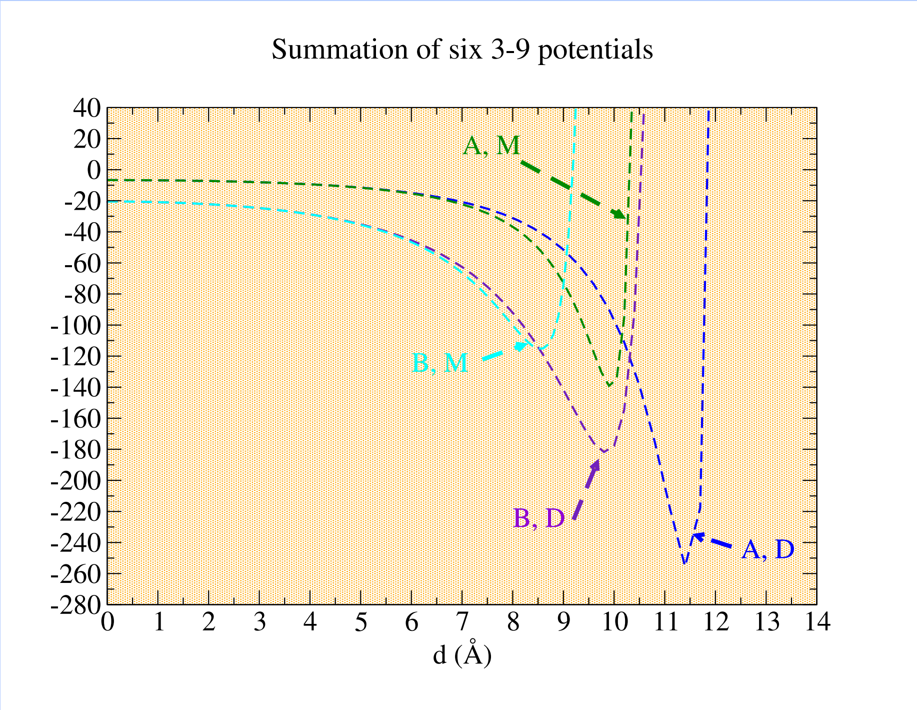

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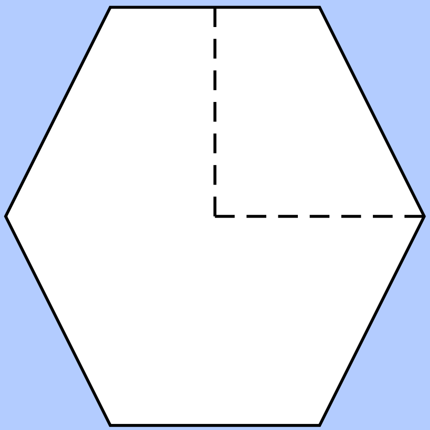
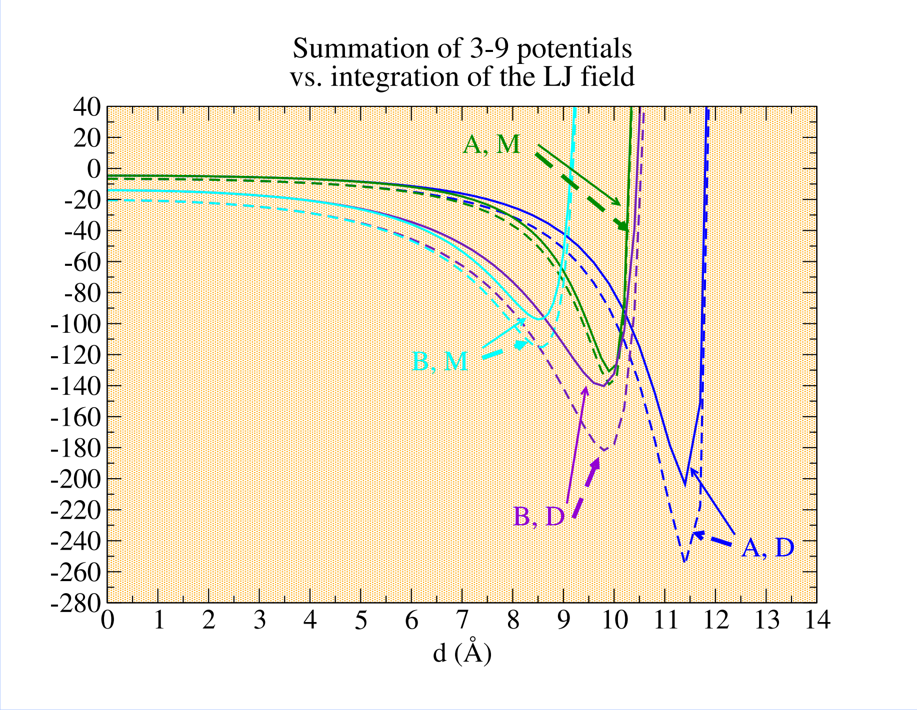
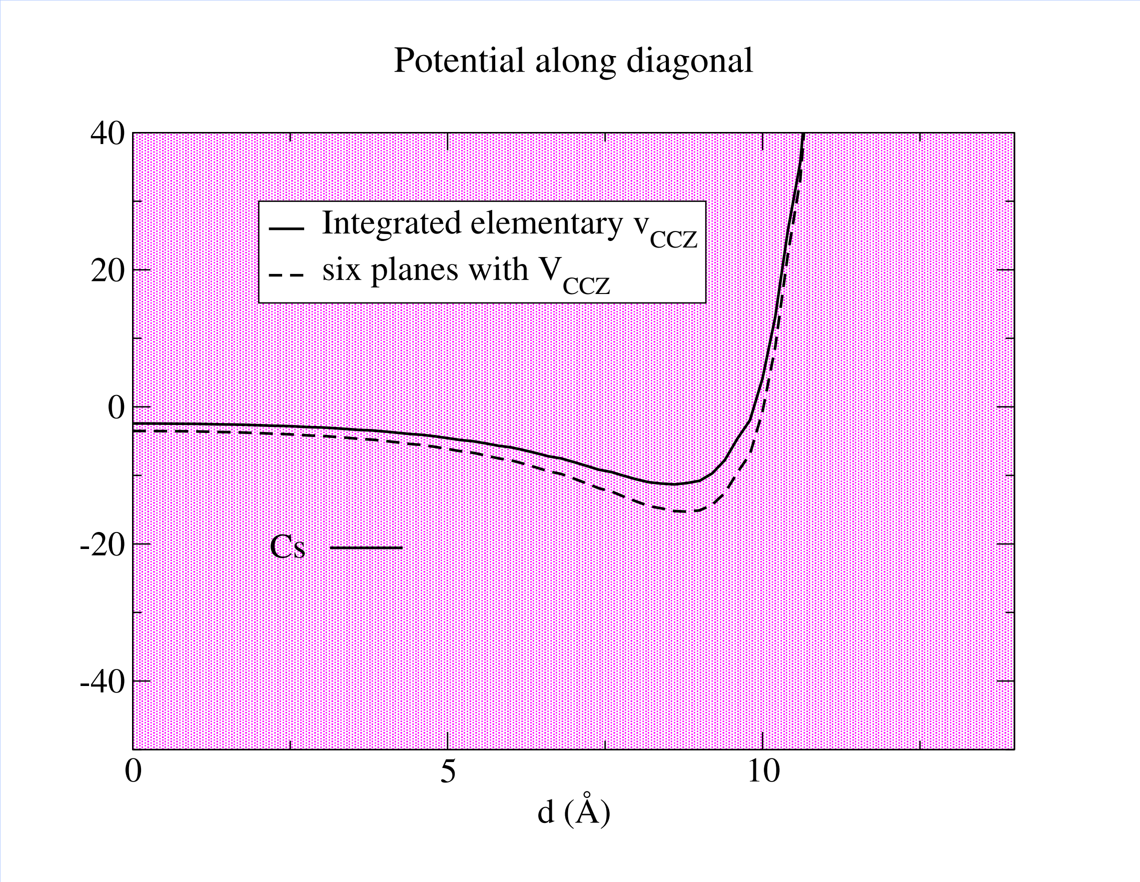




Metallic hexagonal pores



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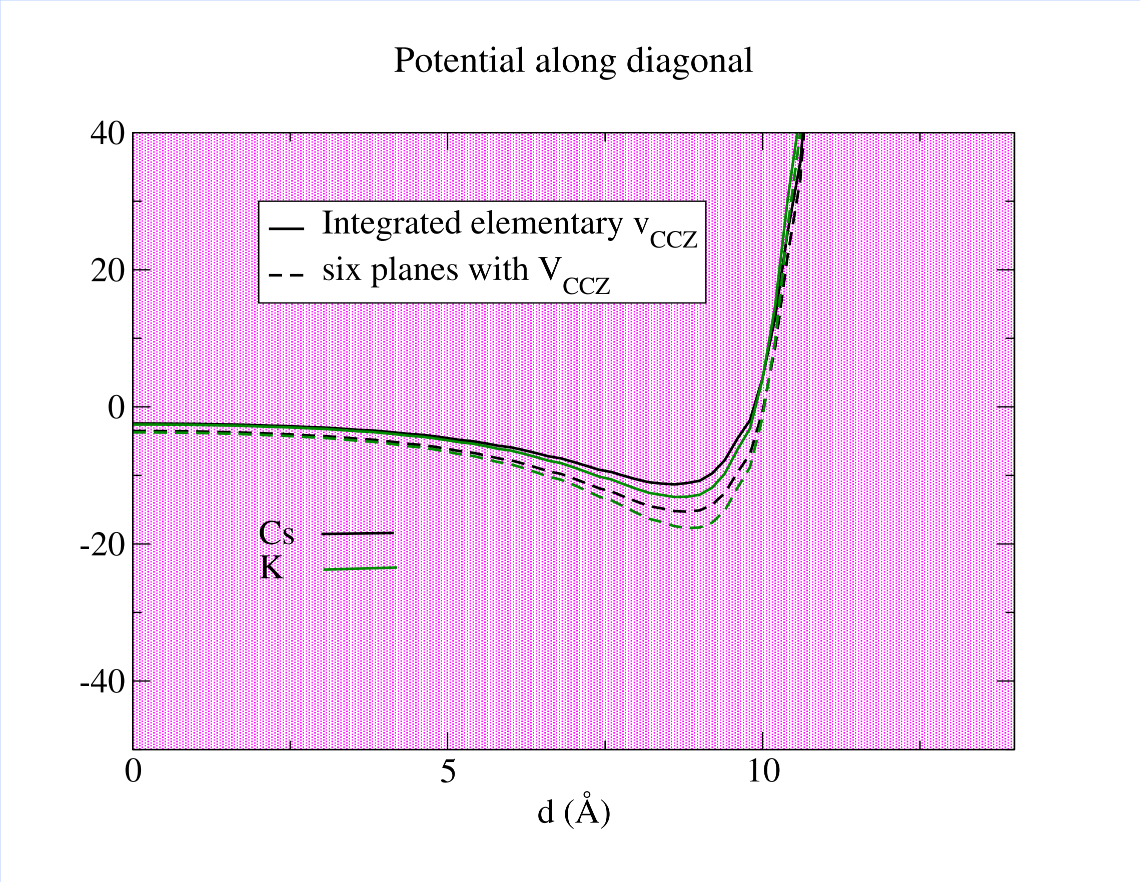

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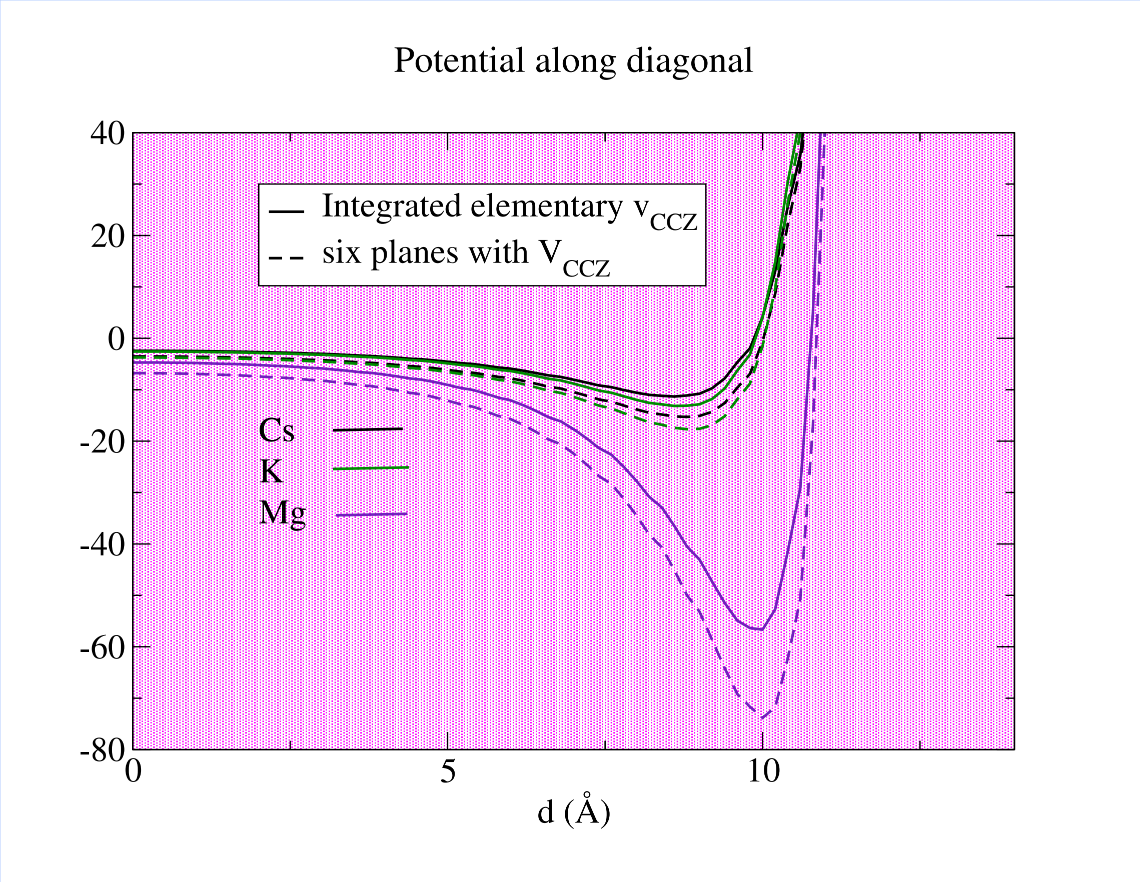

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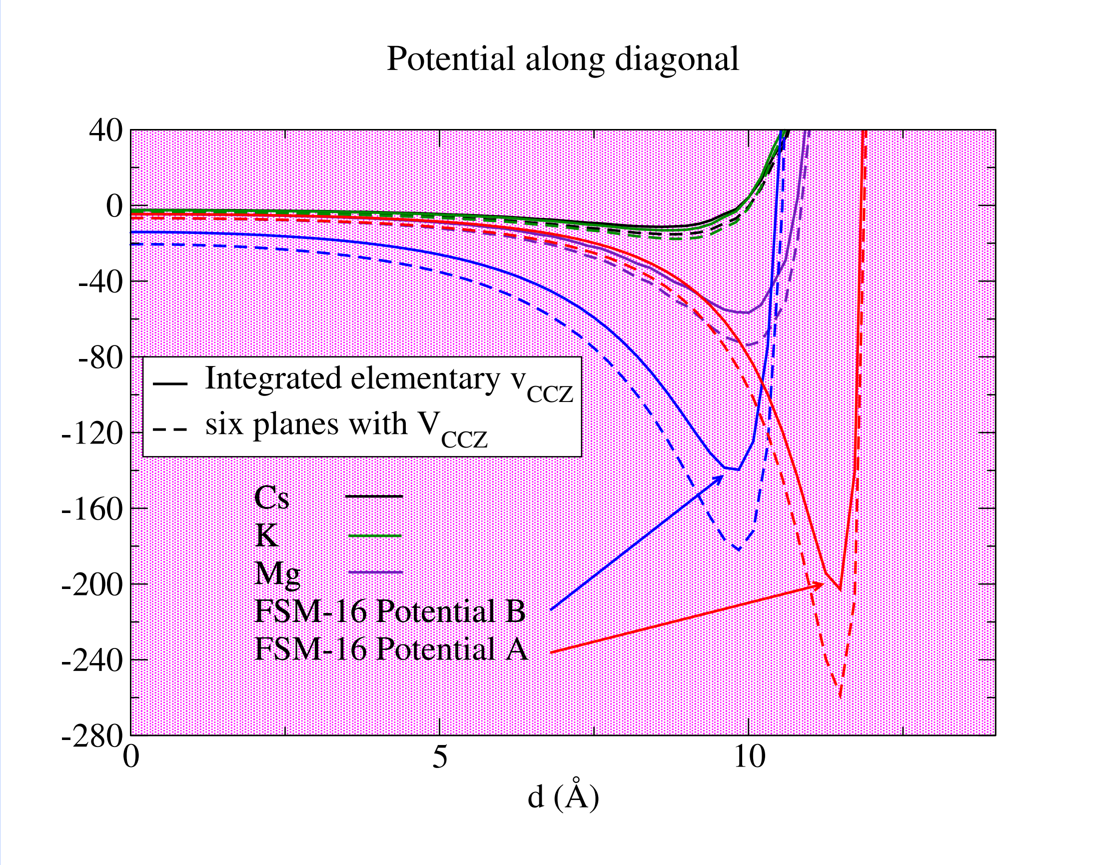

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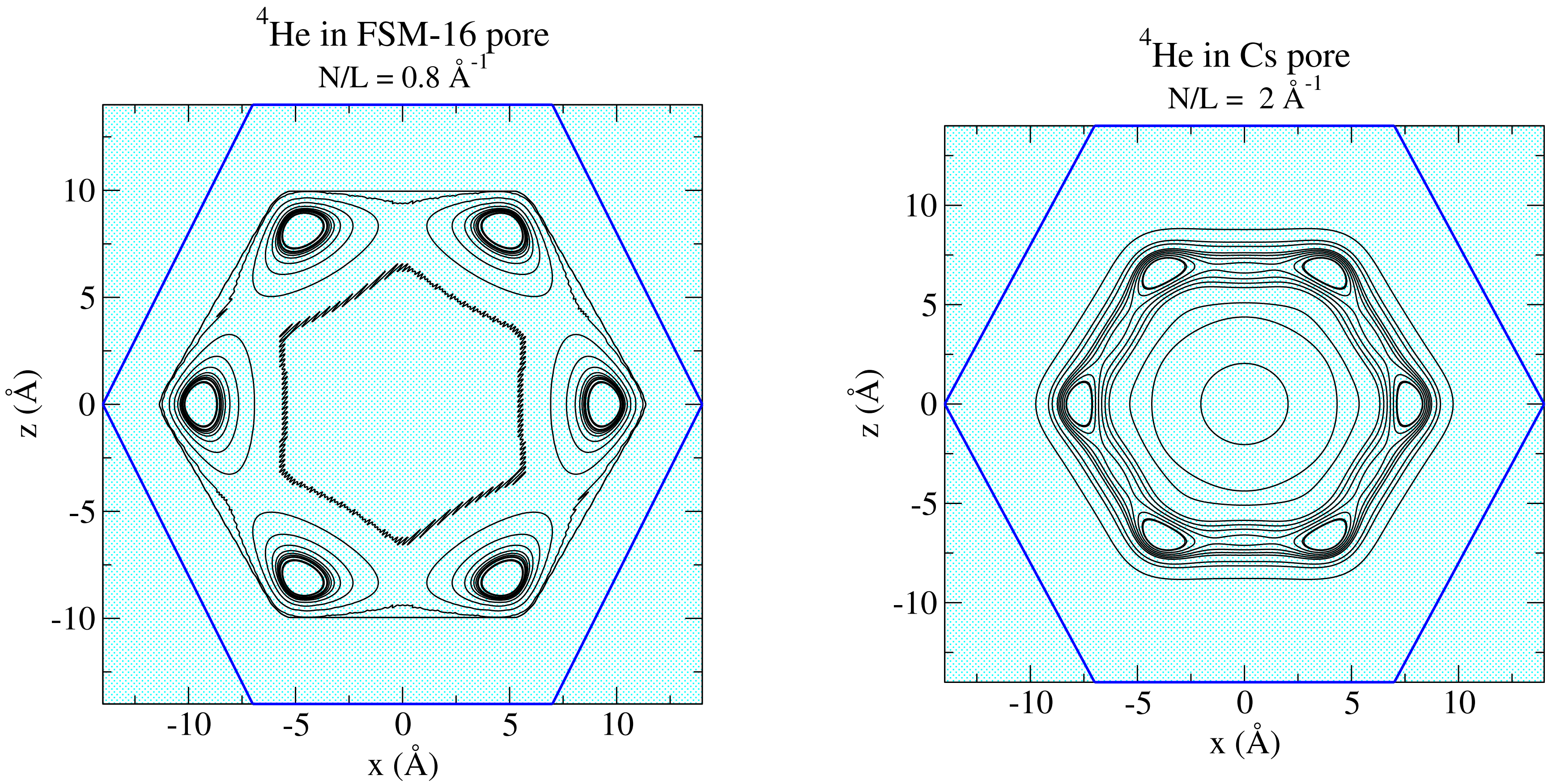
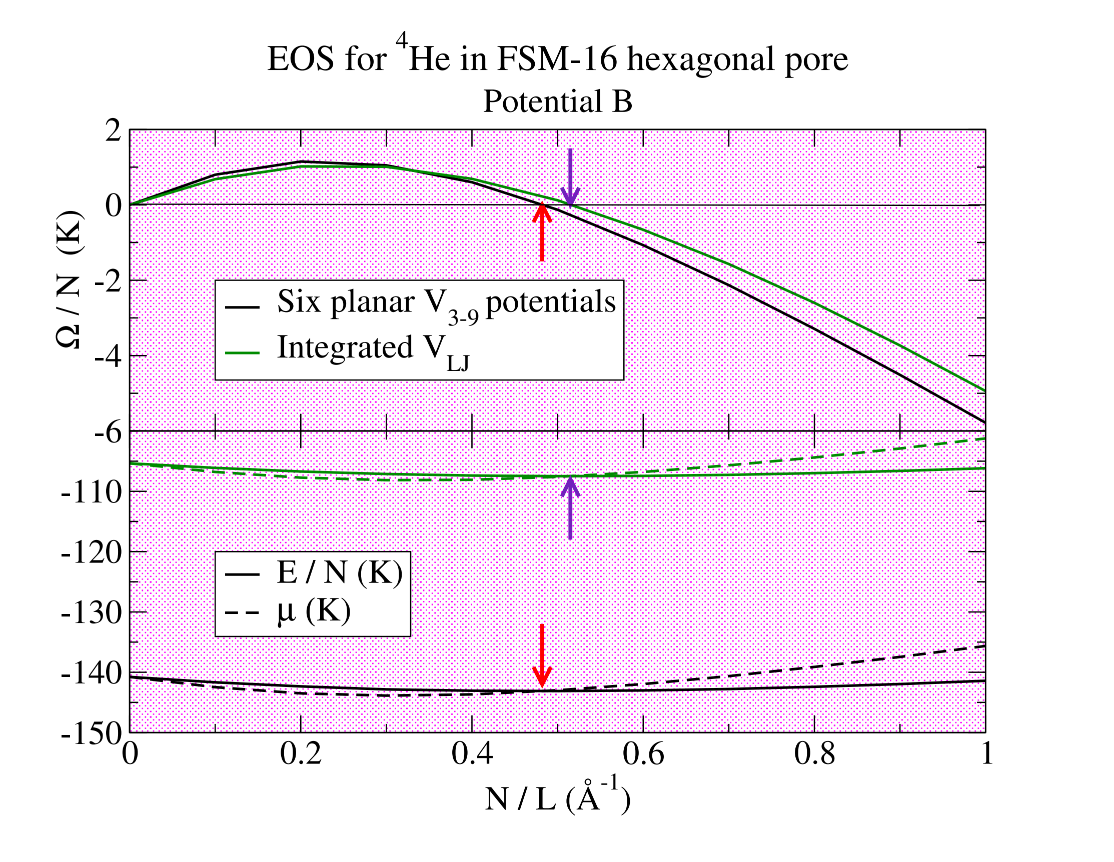
gives

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\rho) + V_s(x,z)\right] \sqrt{\rho(x,z)} = \mu \sqrt{\rho(x,z)}$$

Some density profiles obtained with DFT



Some EOS computed with DFT



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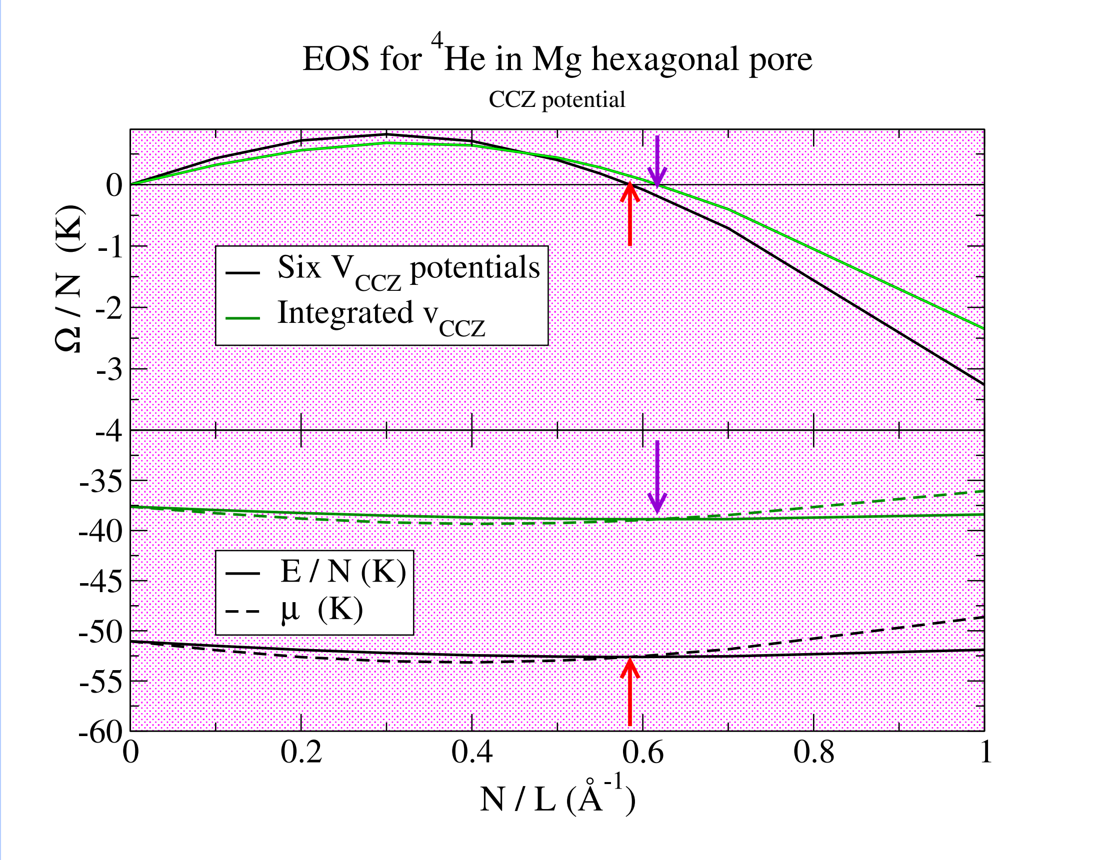

Some energetics

$SUBSTRATE$	$\varepsilon_{\sum}(K)$	$\varepsilon_{\int}(K)$	$\frac{\varepsilon_{\sum}-\varepsilon_{\int}}{\varepsilon_{\int}}$
$FSM--16, A$	-178.36	-135.98	0.31
$FSM--16, B$	-140.77	-105.36	0.34
Mg	-51.04	-37.62	0.36
Li	-23.98	-17.22	0.39
Na	-16.35	-11.58	0.41
K	-10.41	-7.24	0.44
Rb	-9.45	-6.54	0.44
Cs	-9.01	-6.22	0.45

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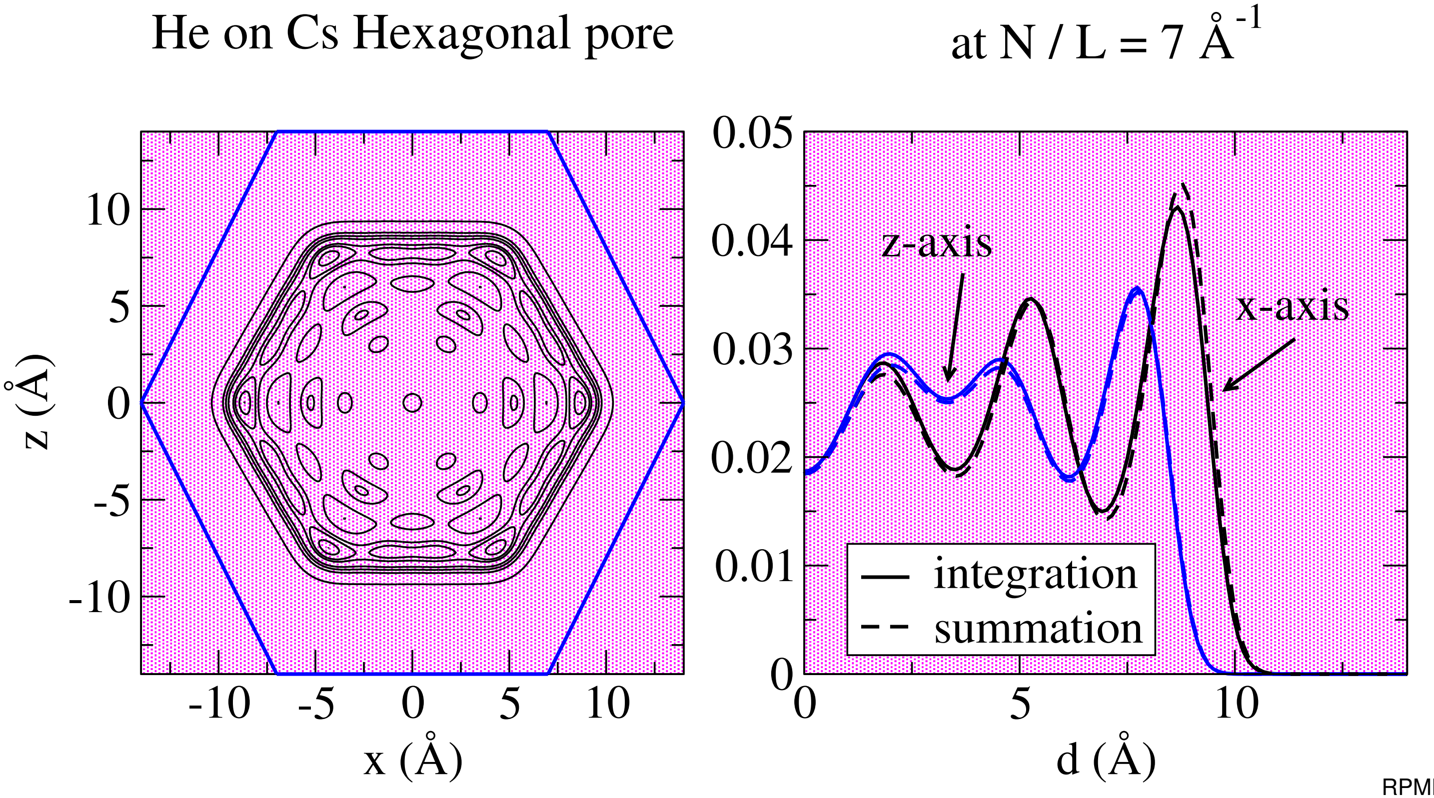
- $\Longrightarrow$ the **He–Cs** system is an interesting laboratory for experimenting on wetting physics.

Some comparison among methods



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- Nextcoming release (RPMBT15 and/or earlier meetings): Condensation of ^{4}He in polygonal and curved pores in 2D and 3D at zero and finite temperatures.