Nanocrystals in the Kitchen

Thomas Fernique

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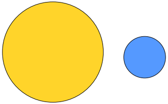
Our running example:
Disks of diameter 1 and $r := \sqrt{2} - 1$:



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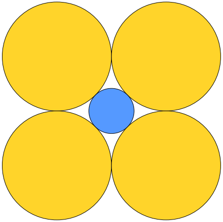

This ratio allows a small disk to exactly fit between four large ones.

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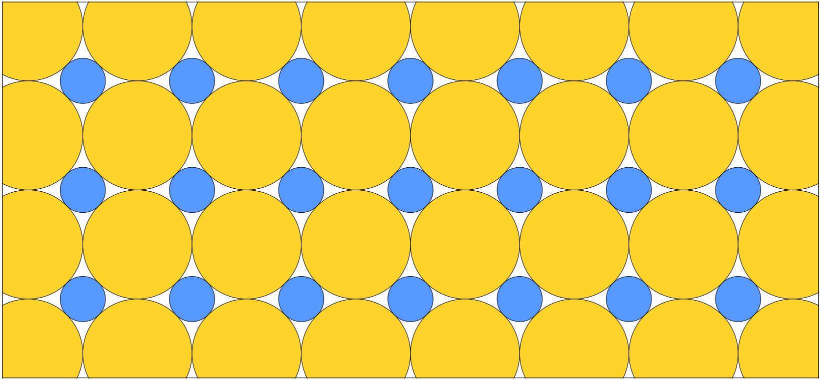

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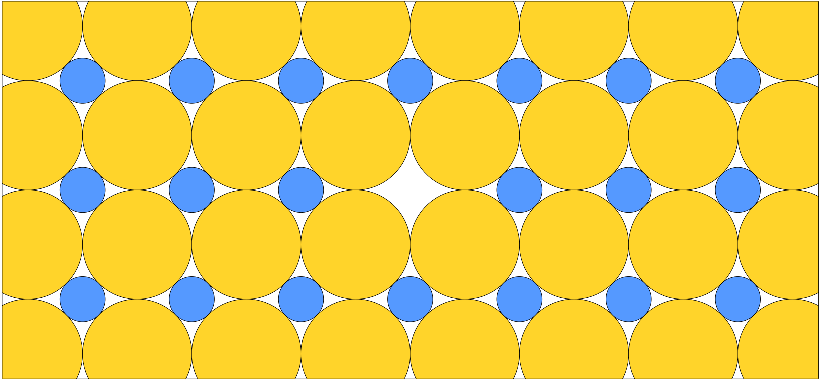

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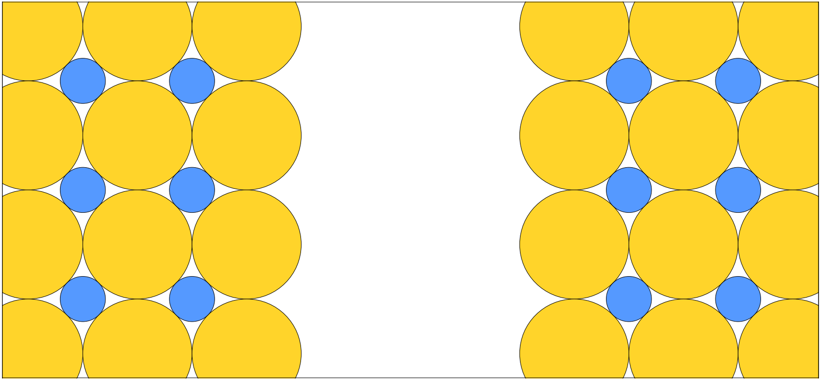

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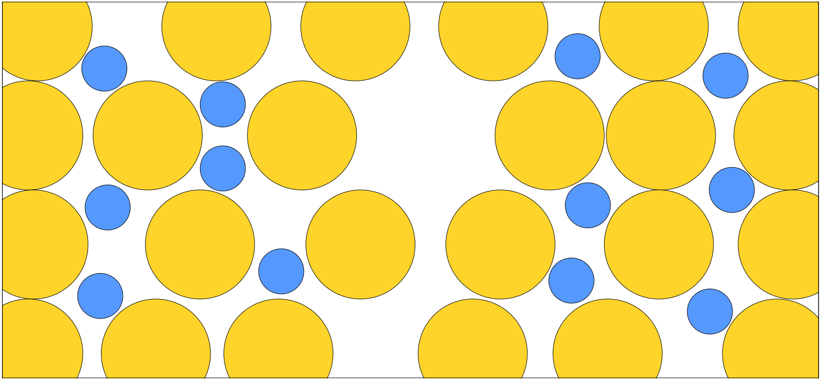

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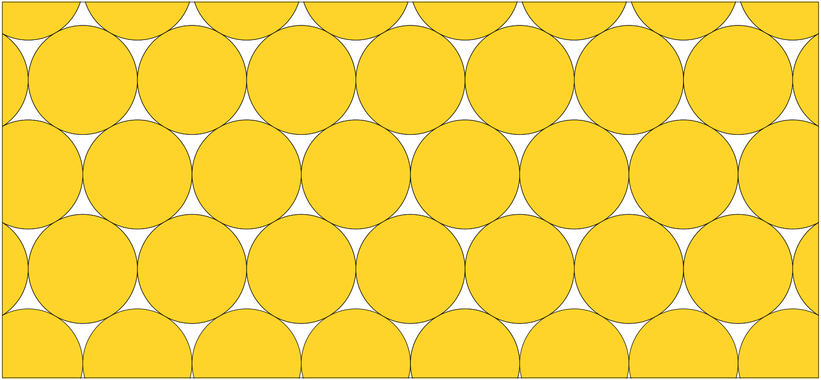

The Hexagonal Compact Packing (HCP) has density $\frac{\pi}{2\sqrt{3}} \leq 91\%$.

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The densest triangle which connects the centers of equal disks connects three pairwise adjacent disks.

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Proof idea: "spread" the density to lower it everywhere below δ^*.

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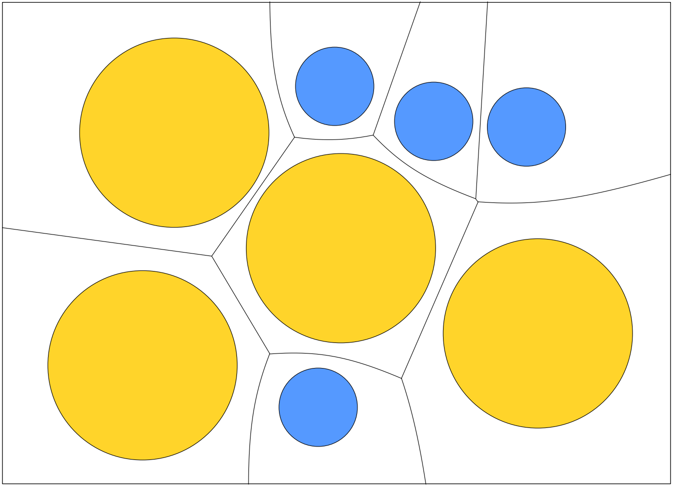
4. show, for every triangle T of $\mathcal{T}$:

$$\sum_{v \in T} U_v(T) \leq E(T), \tag{2}$$

where $E(T) := \delta^* \mathrm{vol}(T) - \mathrm{cov}(T)$ is the emptiness of T.

Step 1: Delaunay triangulation



Points closer to a disk than to any other one ⇝ Voronoï partition.

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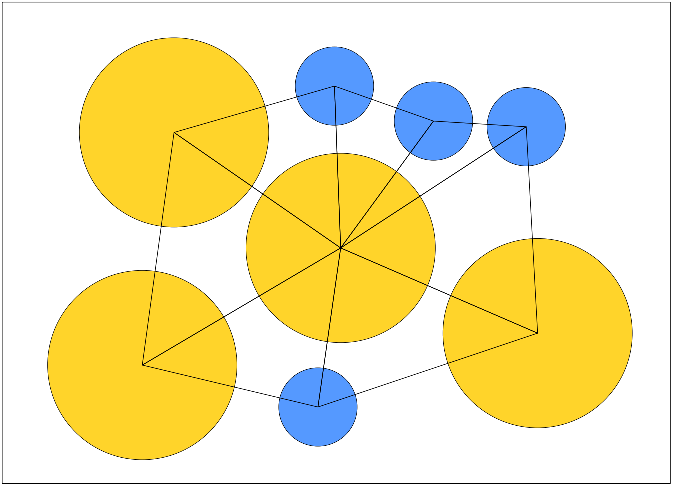

Dual of the Voronoï partition ⇝ Delaunay triangulation.

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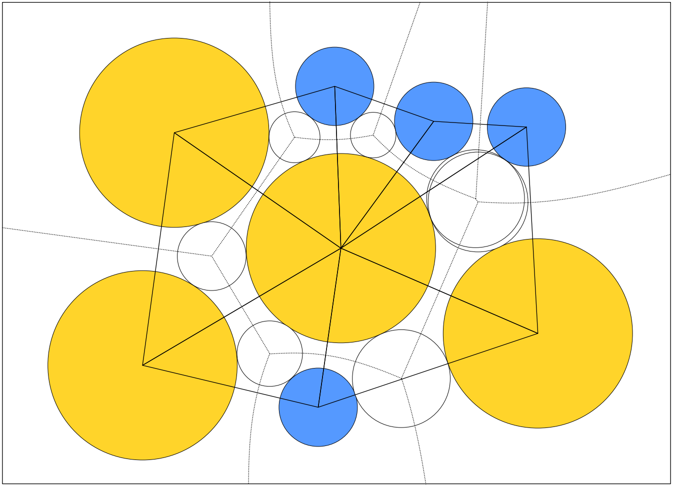

Partition vertex: center of a disk interior-disjoint from the packing.

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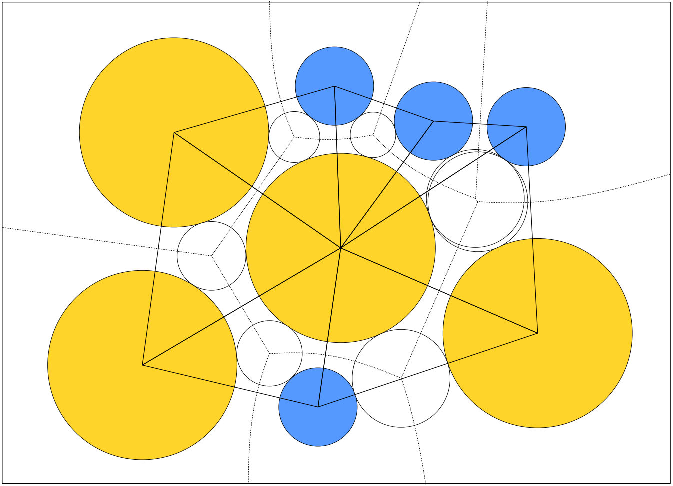
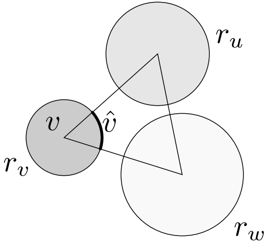


Claim: saturation $\Rightarrow$ edge lengths $\leq 2 + 2r$ and angles $\geq 33^\circ$.

Step 2: Vertex potential



If T connect the centers u, v and w of disks of size r_u, r_v and r_w:

$$U_v(T) := U^*_{r_u r_v r_w} + m\,|\hat{v} - \hat{v}^*|\,,$$

where:

- $\hat{v}$ is the angle in v of T and $\hat{v}^*$ in its tight version T^*;
- $U^*_{r_u r_v r_w} = U^*_{r_w r_v r_u} \in \mathbb{R}$ is the base vertex potential (to be fixed);
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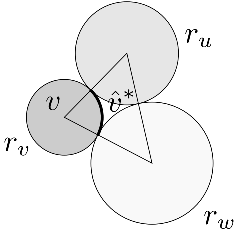

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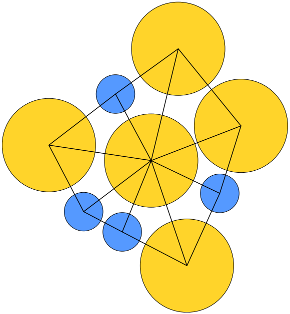
$\sum_{T \ni v} U_v(T) \geq 0.$



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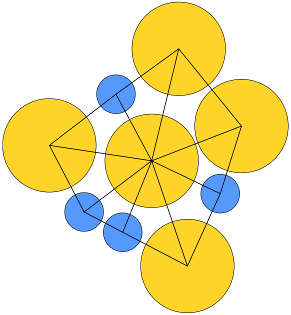

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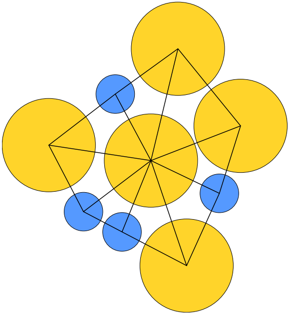

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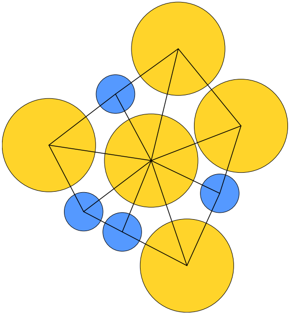

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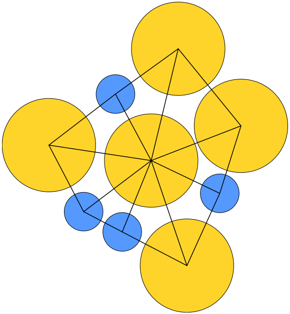

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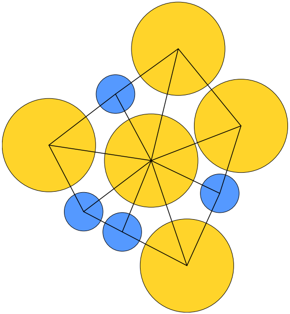

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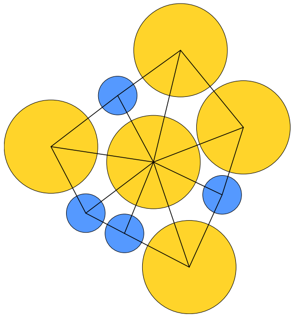

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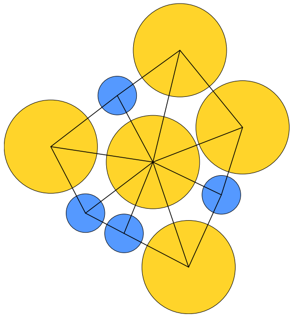

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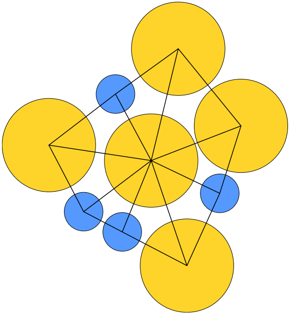

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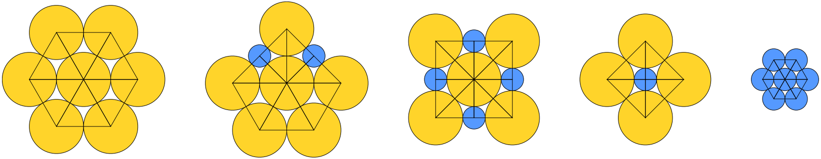

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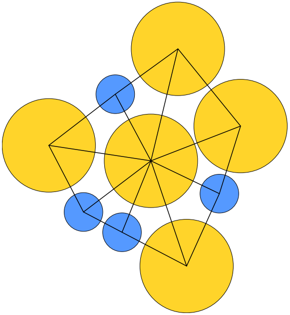

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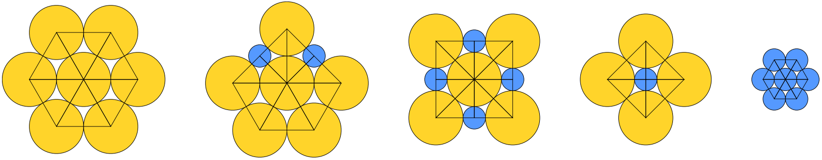

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We also want:

$$\sum_{v \in T} U_v(T) \leq E(T) = \delta^* \mathrm{vol}(T) - \mathrm{cov}(T).$$

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Use the Mean Value Theorem (and, again, Interval Arithmetic).

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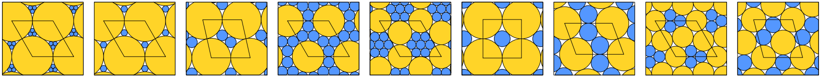

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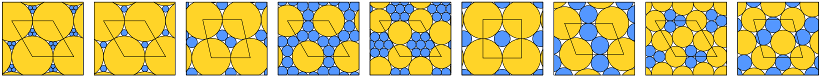

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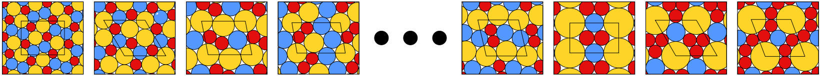

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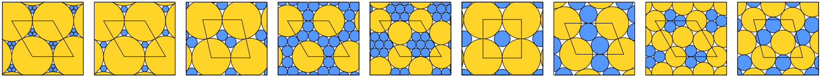

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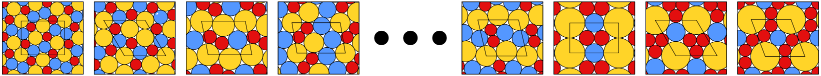

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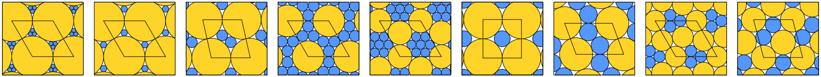

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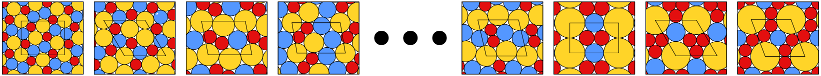

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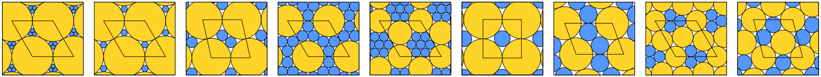

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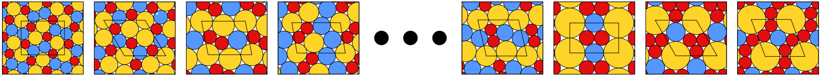

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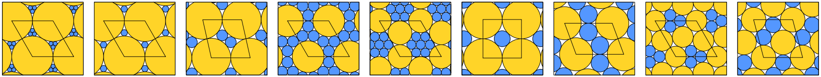

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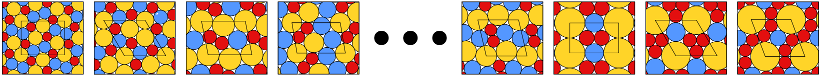

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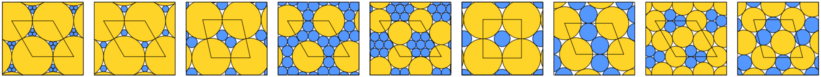

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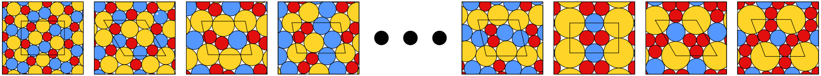

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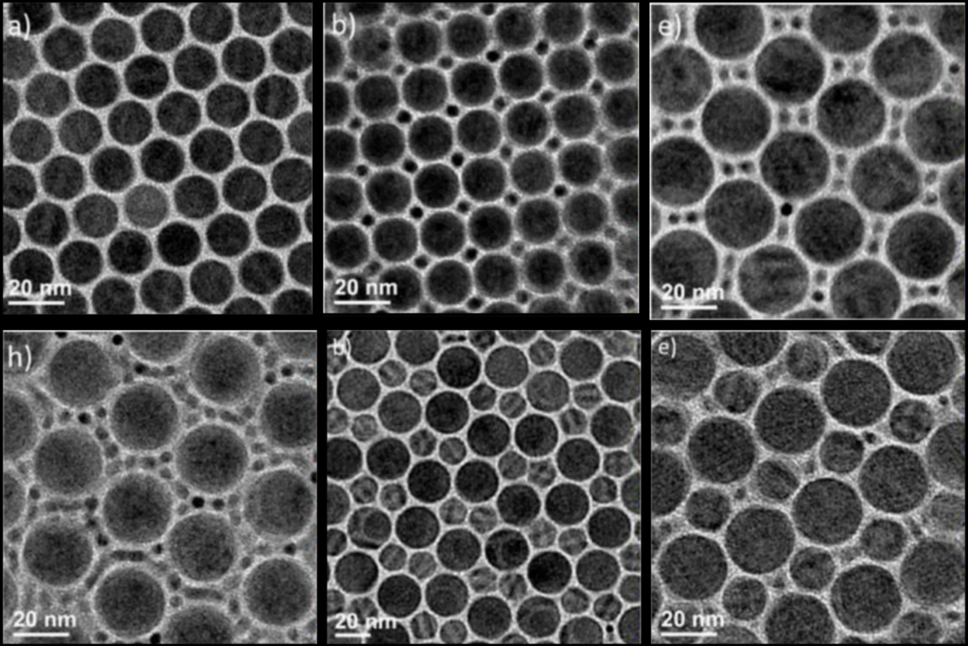
- The case of spheres of size 1 and $\sqrt{2}-1$ should be easier!
- Motivation: material sciences (nanocrystals).


a)
20 nm
b)
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