Searching Novel Higher-κ Dielectric Materials Through High-throughput *Ab Initio* Approach

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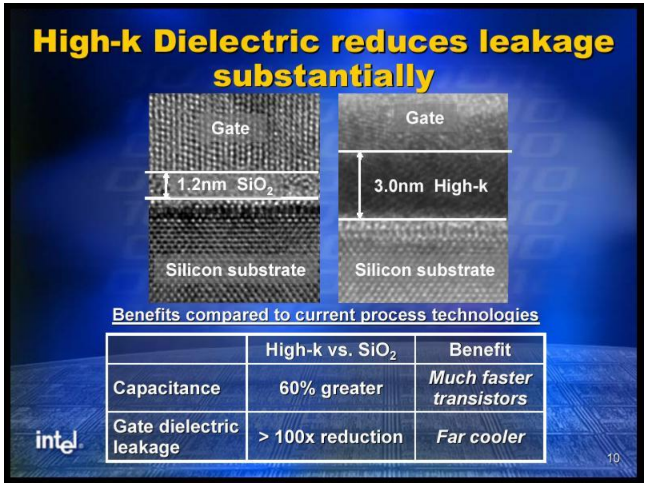
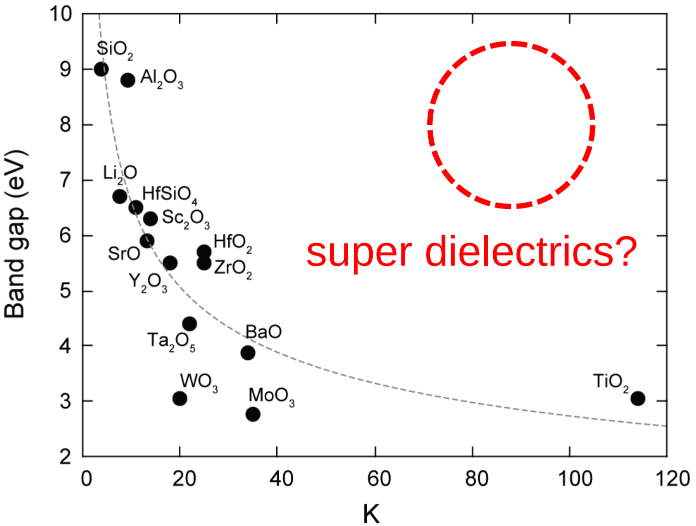
High throughput for new high-k materials



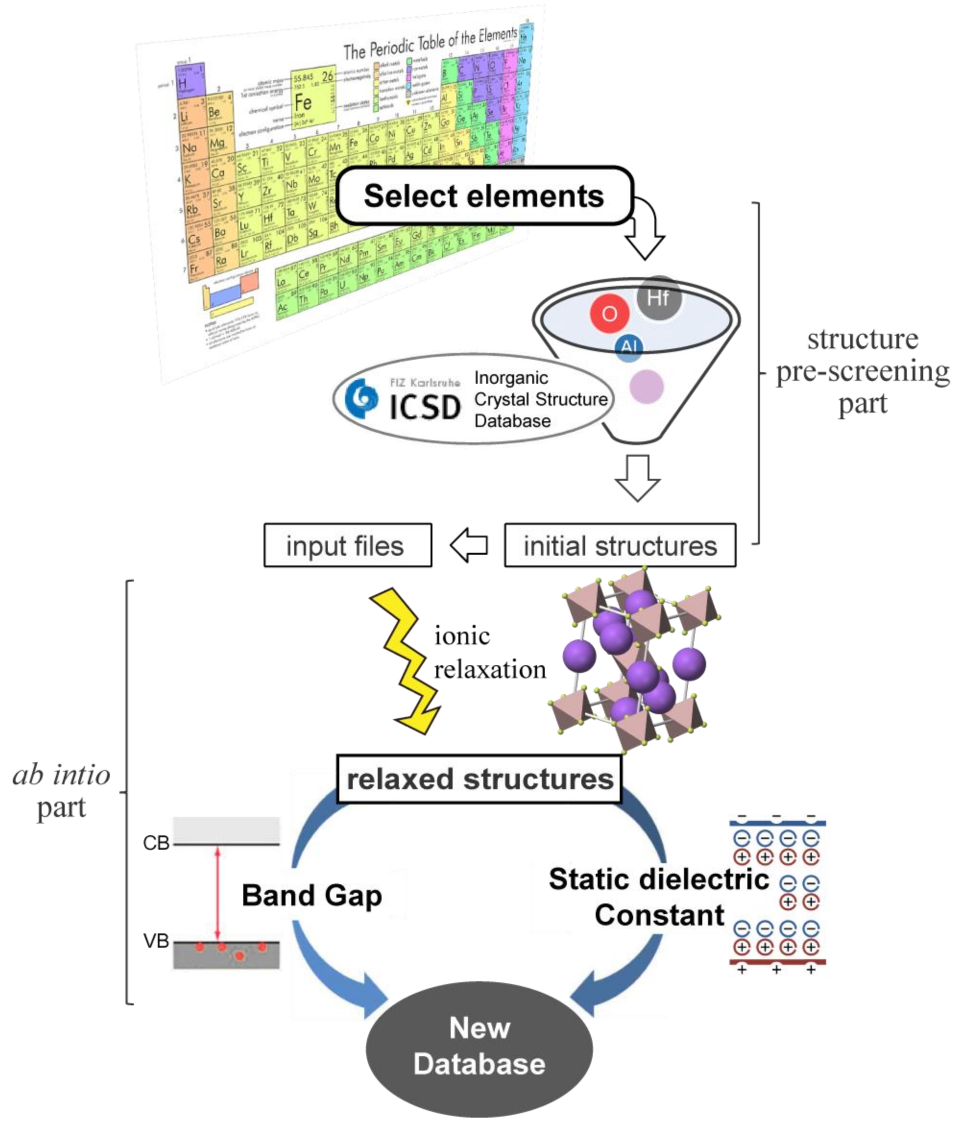
- Ideal condition of high-k dielectrics

: Large permittivity(κ) and large band gap(E_g)



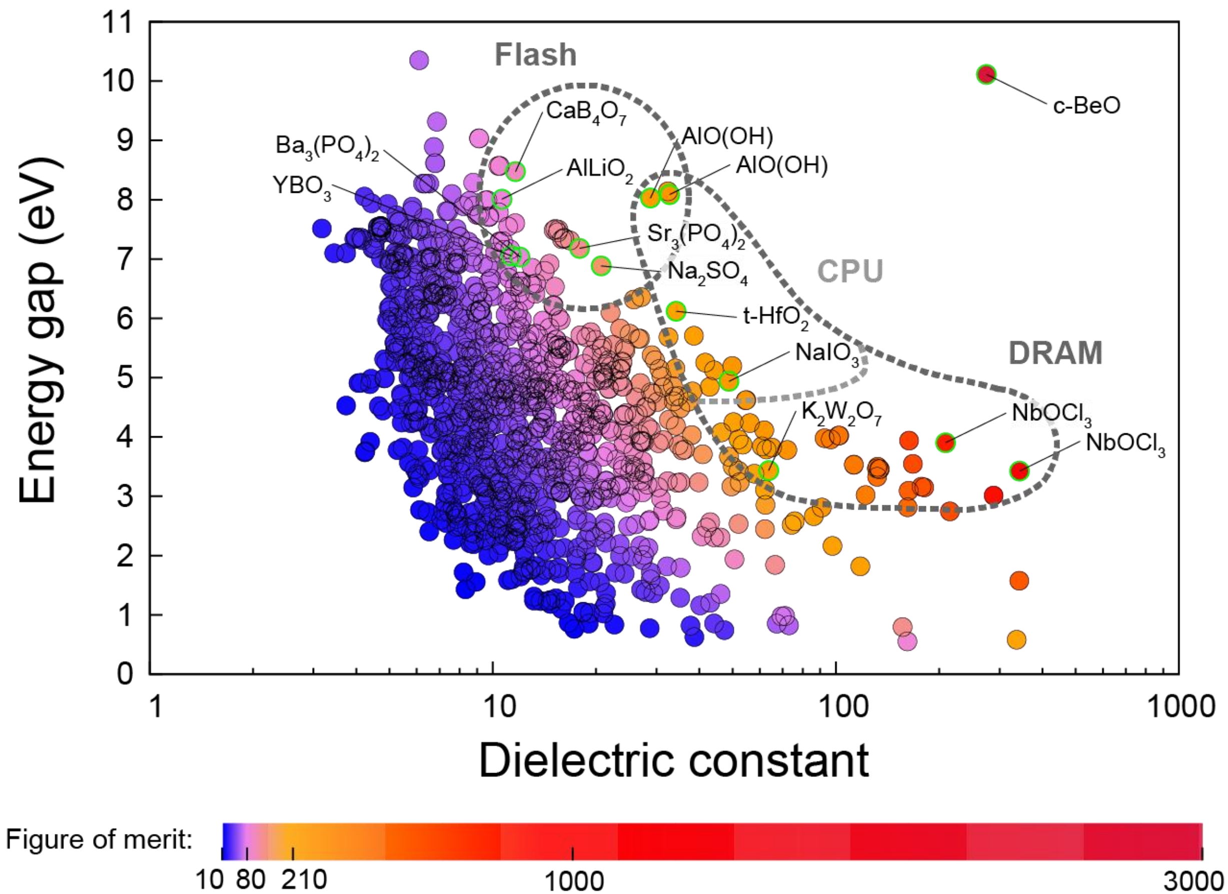
Permittivity vs. band gap (experiment)

- Automation for High-throughput calculation



III. Result: Materials map for high-k dieletrics

- Property Map of ~1,800 oxides
  (metallic and unstable data are excluded on the map)



[DRAM]
- $f_{FOM} > 210$
- $E_g > 3$ eV and $\kappa > 30$

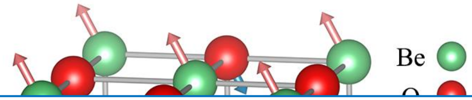
[CPU]
- $f_{FOM} > 210$
- $E_g > 4$ eV
- $E_{vac} > 5.6$ eV

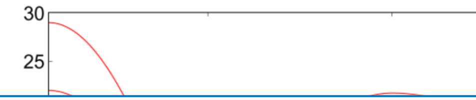
[Flash]
- $f_{FOM} > 80$
- $E_g > 6$ eV

Figure of merits of leakage current : $f = E_g \cdot \kappa$ (approximated)

III. Result: New high-k candidate materials

- c-BeO (rocksalt, high pressure)





- **Two common features for ternary higher-k candidates**

① **Cations in edge-shared octahedra cage**
  - ✓ Edge-shared anion octahedra form loose cages.
  - ✓ Cations in the cages vibrate with soft phonon frequency.

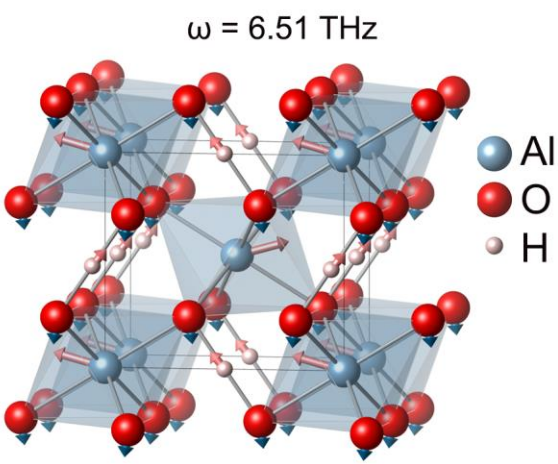
② **Channeled structure by strong covalent oxide unit**
  - ✓ Strong covalent oxide unit + loosely bound cation
  - ✓ Channeled structure : ions easily vibrate along the channel that is not blocked by other ions.

- AlO(OH)

ε^{∞} : 3.2

ε^{0} : 32.8

E_g : 8.1 eV



- Na_2SO_4

ε^{∞} : 2.3

ε^{0} : 20.7

E_g : 6.9 eV