DFT Computer Simulations of High-k Materials for Future Semiconducting Devices

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Research question:

How can employing VASP simulations for analyzing the static dielectric properties of high-k materials aid in the streamlining discovery process and identification of other ideal high-k materials with enhanced capacitance for future semiconductor applications?

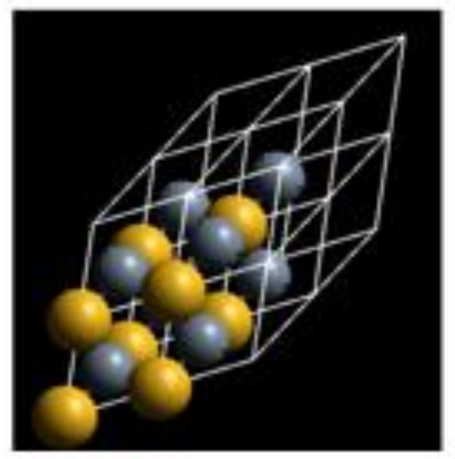
Background:

• The Creating Helpful Incentives to Produce Semiconductors for America Act (CHIPS & Science Act), facilitates the resources for innovation, exploration, & growth in the semiconductor industry.

• Recent advancements in semiconductor technology has led to miniaturization of electronic devices, requiring faster & more efficient performance than SiO2.

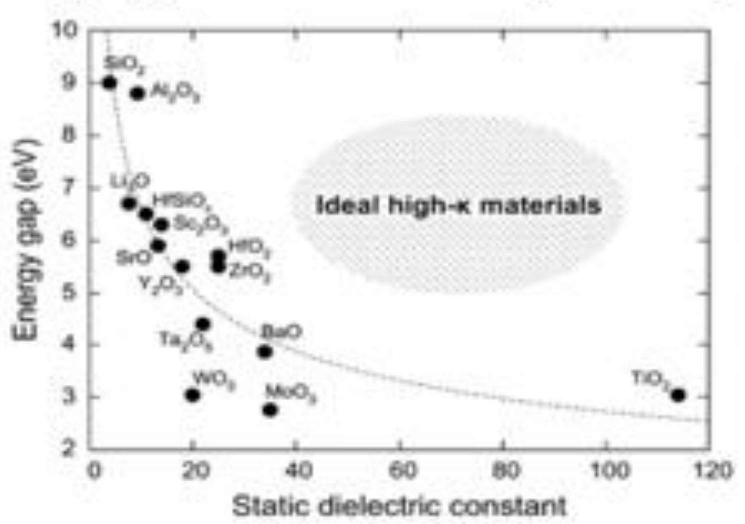
• High-k dielectric oxides/materials have emerged as a promising material to enhance the performance and scaling down of semiconducting devices.

• High-k oxides enable higher capacitance, leading to reduced leakage and power consumption as well as faster processing speeds and increased functionality.



SiC projected in VASP:
https://www.vasp.at/wiki/index.php/Dielectric_properties_of_SiC

Ideal high-k material Graph:
https://www.nature.com/articles/am201557



• VASP outputs for dielectric tensor calculated in the independent-particle (IP) calculation excluding and including local field effects.

```
HEAD OF MICROSCOPIC STATIC DIELECTRIC TENSOR (INDEPENDENT PARTICLE, excluding Hartree and local field
effects)
------------------------------------------------------
         7.135462    -0.000000     0.000000
        -0.000000     7.135462    -0.000000
         0.000000    -0.000000     7.135462
------------------------------------------------------

MACROSCOPIC STATIC DIELECTRIC TENSOR (including local field effects in DFT)
------------------------------------------------------
          6.894122     0.000000    -0.000000
         -0.000000     6.894122     0.000000
          0.000000    -0.000000     6.894122
------------------------------------------------------

BORN EFFECTIVE CHARGES (including local field effects) (in |e|, cummulative output)
---------------------------------------------------------------------
ion    1
    1     2.70352    -0.00000     0.00000
    2    -0.00000     2.70352    -0.00000
    3     0.00000     0.00000     2.70352
ion    2
    1    -2.70352     0.00000    -0.00000
    2     0.00000    -2.70352     0.00000
    3    -0.00000    -0.00000    -2.70352
```

• Ionic Contributions to the Static Dielectric Properties

```
MACROSCOPIC STATIC DIELECTRIC TENSOR IONIC CONTRIBUTION
------------------------------------------------------
          3.308948    -0.000000     0.000000
         -0.000000     3.308948    -0.000000
          0.000000    -0.000000     3.308948
------------------------------------------------------

ELASTIC MODULI CONTR FROM IONIC RELAXATION (kBar)
Direction    XX          YY          ZZ          XY          YZ          ZX
--------------------------------------------------------------------------------
XX          -0.0000     -0.0000     -0.0000      0.0000      0.0000     -0.0000
YY          -0.0000     -0.0000      0.0000      0.0000     -0.0000      0.0000
ZZ          -0.0000      0.0000     -0.0000      0.0000      0.0000     -0.0000
XY           0.0000      0.0000      0.0000   -266.6739     -0.0000      0.0000
YZ           0.0000     -0.0000      0.0000     -0.0000   -266.6739      0.0000
ZX          -0.0000      0.0000     -0.0000      0.0000      0.0000   -266.6739
--------------------------------------------------------------------------------

PIEZOELECTRIC TENSOR IONIC CONTR  for field in x, y, z        (C/m^2)
         XX          YY          ZZ          XY          YZ          ZX
--------------------------------------------------------------------------------
  x    -0.00000     0.00000    -0.00000     0.00000     0.88391    -0.00000
  y     0.00000    -0.00000     0.00000    -0.00000    -0.00000     0.88391
  z    -0.00000    -0.00000    -0.00000     0.88391     0.00000    -0.00000
```

Methods:

• Ran density-functional theory (DFT) calculations using Vienna Ab initio Simulation Package (VASP) on Arizona State University's supercomputer, Sol.
• VASP requires 4 inputs to construct a simulation which are
INCAR – controls the parameters for the calculation
KPOINTS – discrete points to sample the Brillouin zone
POSCAR – positions of atoms in Cartesian coordinates
POTCAR – Pseudopotentials used for the calculations

ood02.sol.rc.asu.edu/pun/sys/dashboard/files/fs//home/cjlope20/1_SiC/INCAR

```
## This is the standard DFT
## or hybrid functional calculation
ISMEAR =  0
SIGMA  =  0.01
EDIFF  = 1.E-8

## to get the Born effective charges
## and the macroscopic dielectric tensor
LEPSILON = .TRUE.

#LRPA = .TRUE. Not recommended Check source
## ADD LPEAD for faster convergence, w.r.t
## k-point sampling, of LEPSILON=.TRUE.
LPEAD = .TRUE.

## to get the ionic contribution
## to the macroscopic dielectric tensor
#IBRION = 8

## As an alternative to LEPSILON = .TRUE.
## you might try the following:
#LCALCEPS = .TRUE.

## Another option is:
#IBRION = 6
#NFREE = 2
```

• Calculating static dielectric properties done by density functional perturbation theory done in VASP through LEPSILON=.TRUE.

Results/Progress so far:

• Learned how to use VASP to do calculations based on Density Functional Perturbation Theory (DFPT) to determine the static dielectric properties & born effective charges of SiC, Silicon Carbide.
• Future goal is to conduct more VASP simulations on a diverse range of materials, aiming to identify other materials with high static dielectric tensors for potential integration into semiconductor electronics.

Acknowledgements/ References:

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