# Optical and elastic properties of diamond-like carbon with metallic inclusions: a theoretical study

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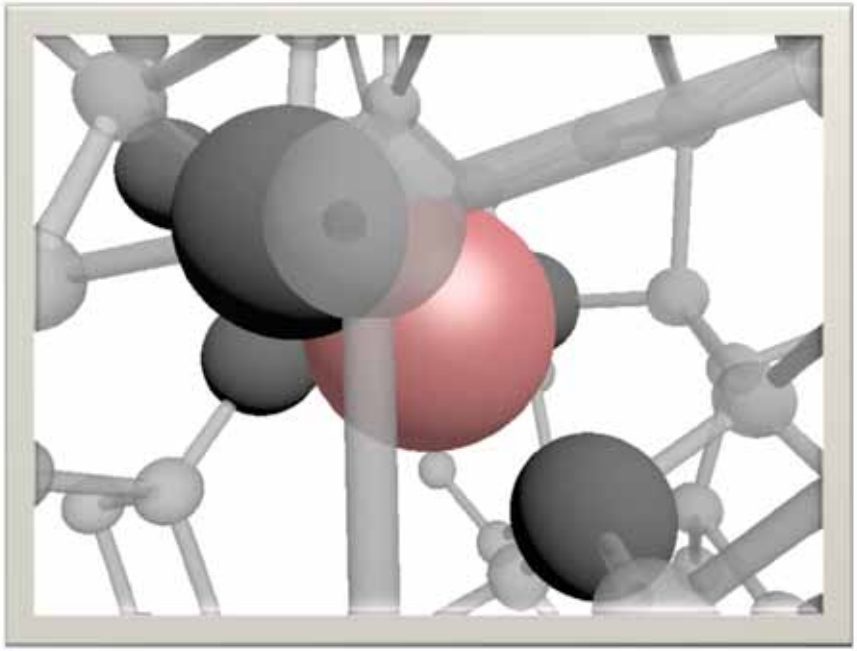
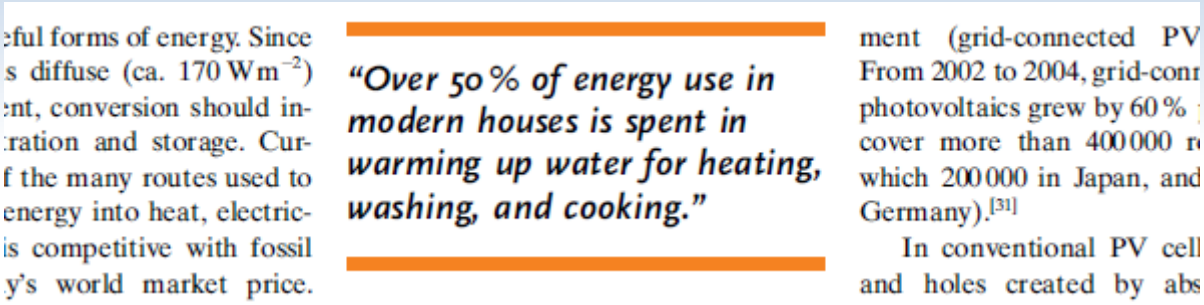
MRS Fall Meeting 2012



# Introduction



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From 2002 to 2004, grid-conn
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In conventional PV cell
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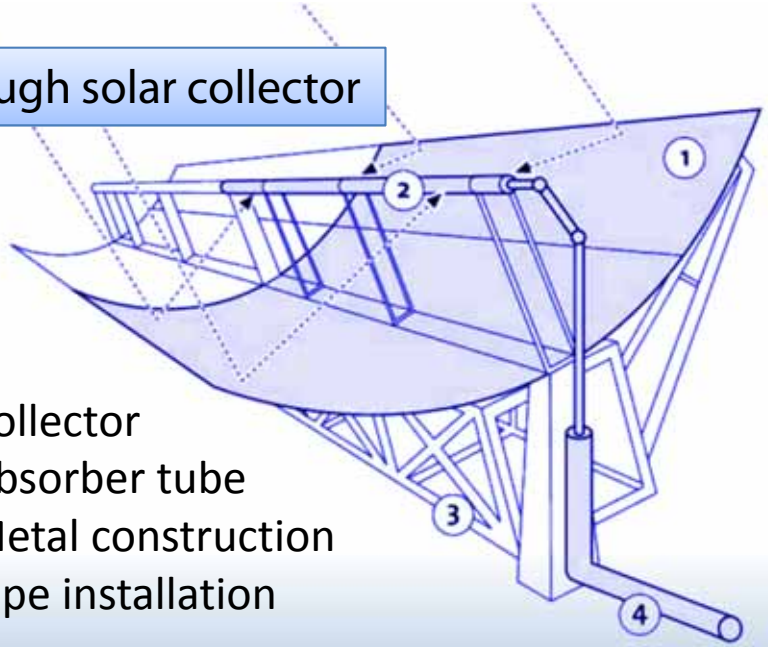
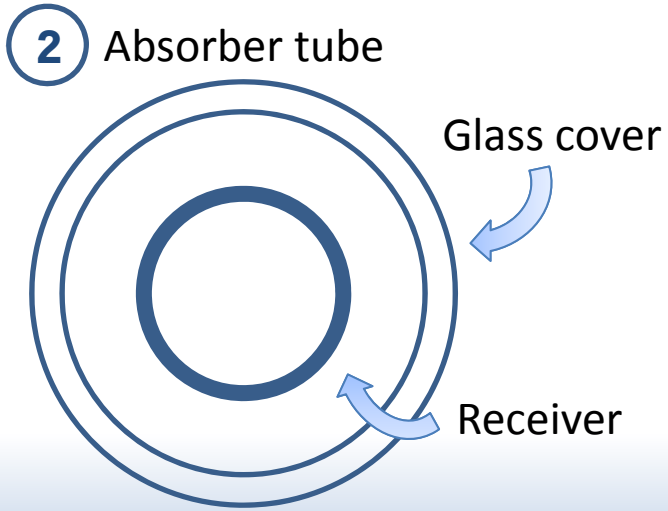
trough solar collector

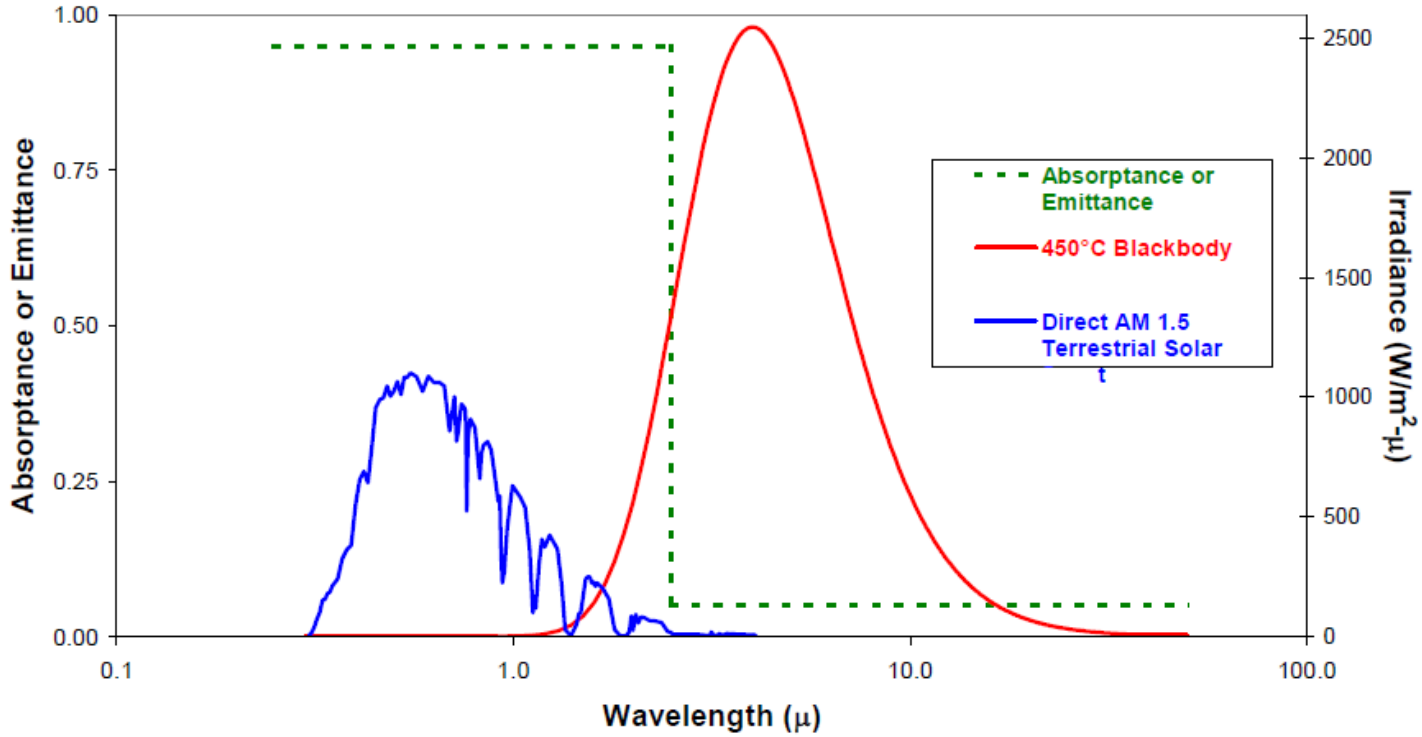



1. Collector
2. Absorber tube
3. Metal construction
4. Pipe installation



# Motivation

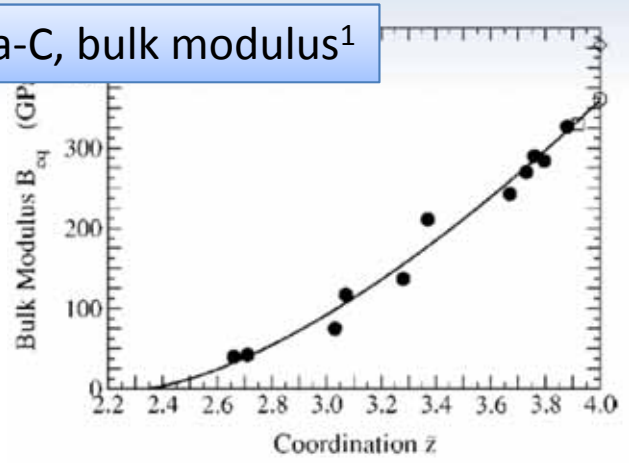
The efficiency of the collector depends crucially on:
the **selectivity** (solar absorbance / thermal emittance), and
the **stability** (high operating temperatures) of the absorber



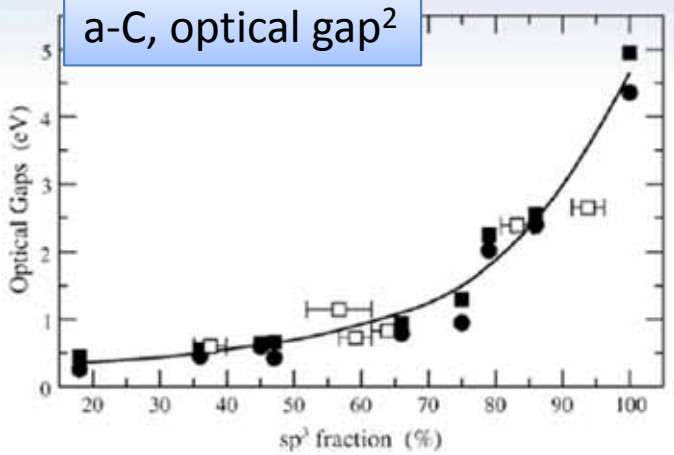
# Diamond-like carbon

Diamond-like carbon (DLC) is tough with suitable optical gap

a-C, bulk modulus[1]




a-C, optical gap[2]




[1]C. Mathioudakis, G. Kopidakis, P. Patsalas, and P.C. Kelires, Diam. Relat. Mater. **16**, 1788 (2007).

[2]C. Mathioudakis, G. Kopidakis, P.C. Kelires, C.Z. Wang, and K.M. Ho, Phys. Rev. B **70**, 125202 (2004).

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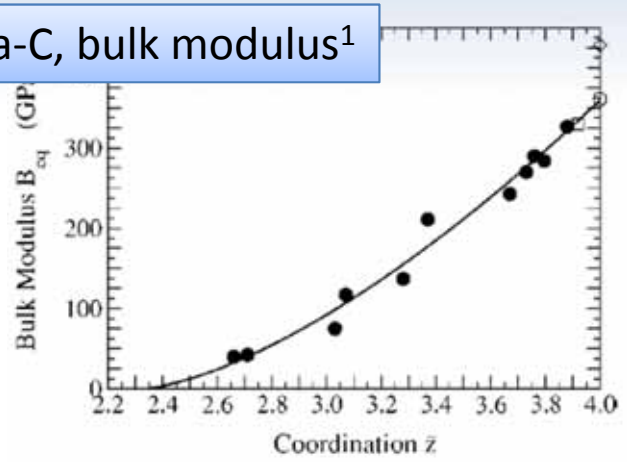
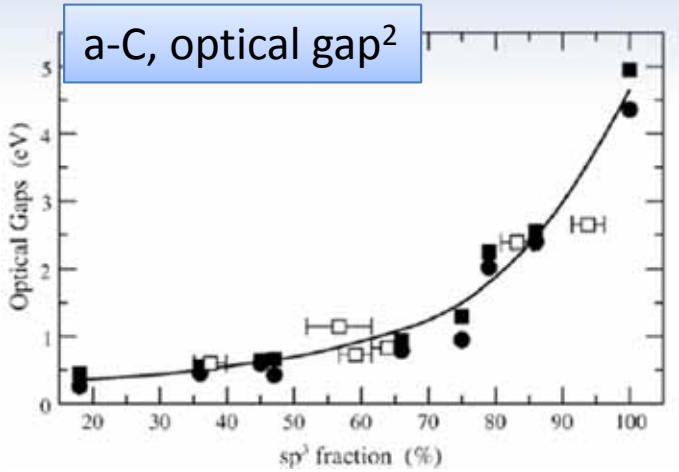
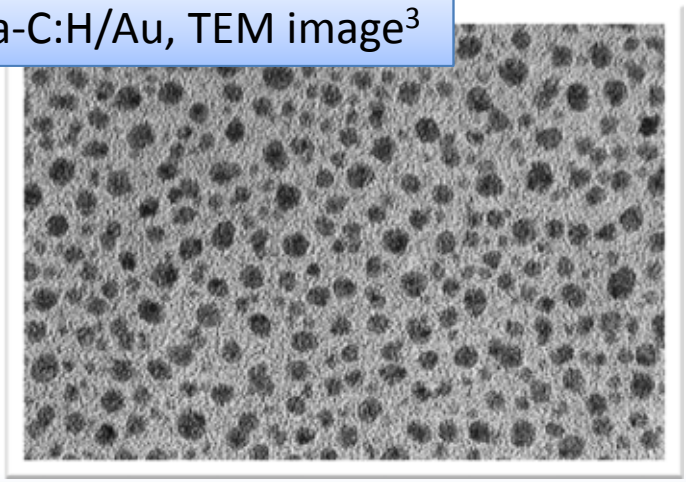


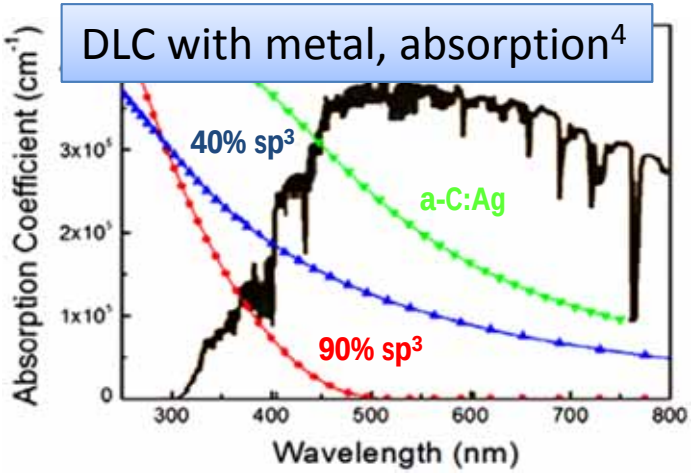

a-C, optical gap[2]




a-C:H/Au, TEM image[3]



DLC with metal, absorption[4]





[1]C. Mathioudakis, G. Kopidakis, P. Patsalas, and P.C. Kelires, Diam. Relat. Mater. **16**, 1788 (2007).
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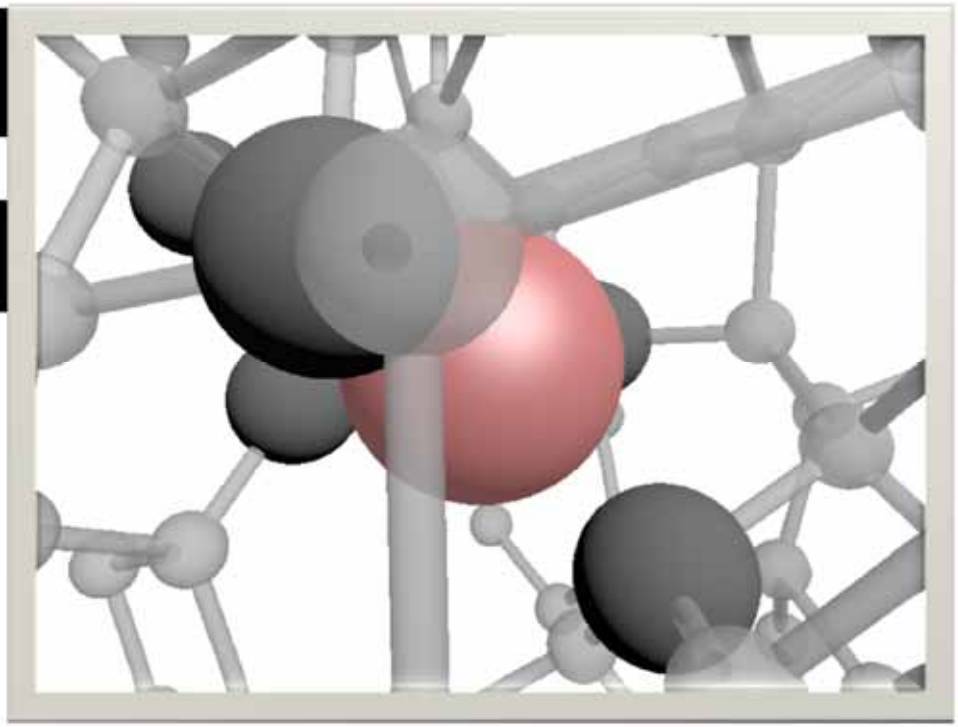
[3]R. Gampp (1996), adapted from P. Oelhafen and A. Schüler, Solar Energy **79**, 110 (2005).
[4]H. Zoubos, G. Constantinidis, D. Pentaras, S. Kalogirou, P.C. Kelires, and P. Patsalas, ICMCTF, San Diego (2011)

# Simulation and design of metal-containing DLC

**Structural models**

**Properties**

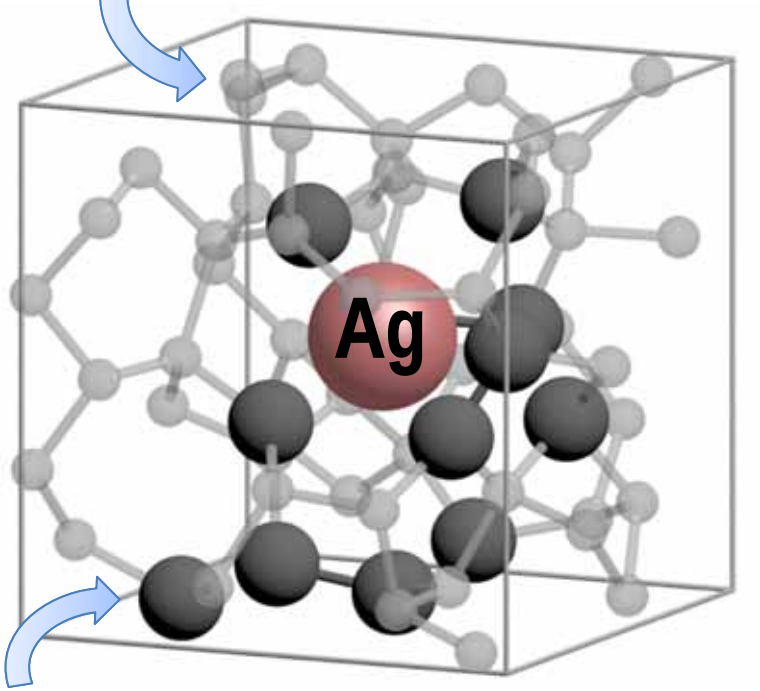
- **Structural**
- **Electronic**
- **Optical**
- **Mechanical**



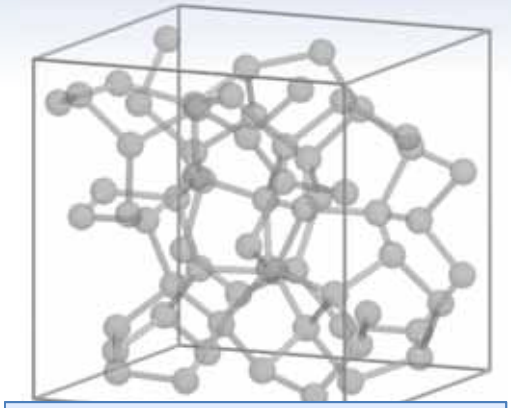
# Structural models

Models of 70-100% $sp^3$ DLC and Ag/Cu-DLC

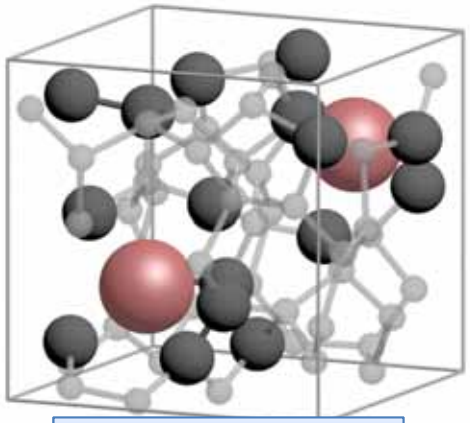
$sp^3$-bonded C




$sp^2$-bonded C



"amorphous diamond"

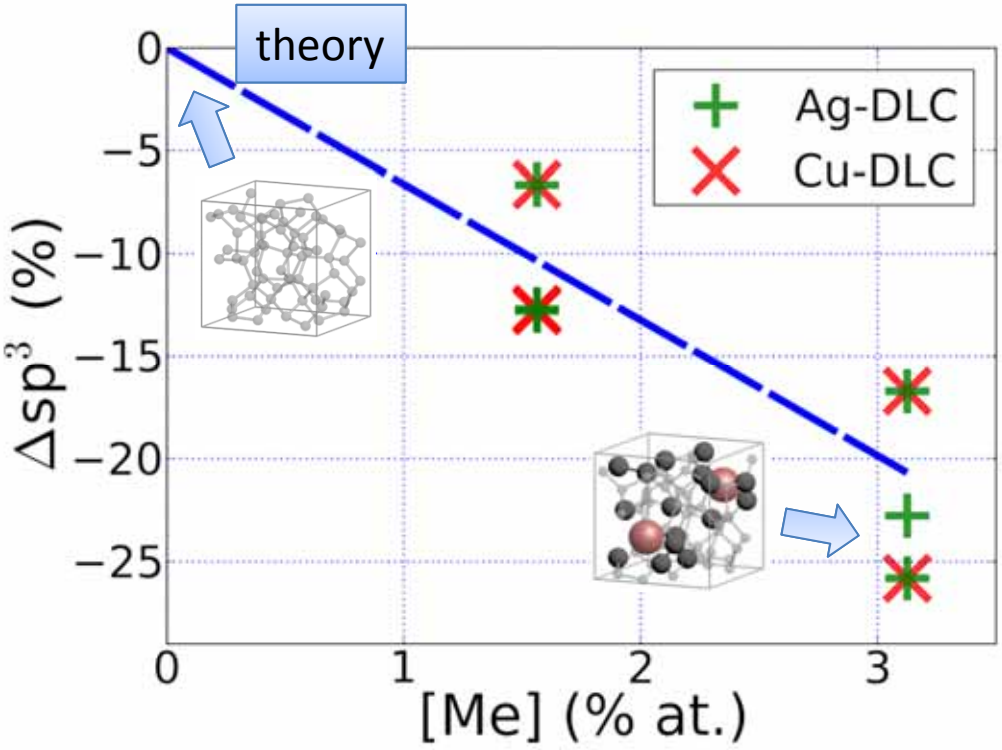


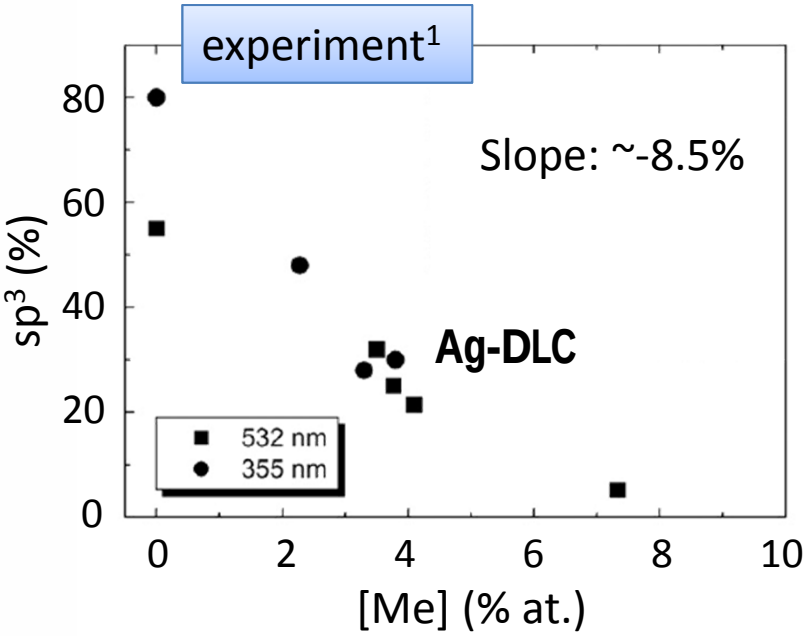
3% at. Me - DLC

PBEsol DFT for structural optimization

# Structural properties

Graphitization of DLC with metal incorporation:
7% decrease in $sp^3$-bonded C for 1% increase in metal content

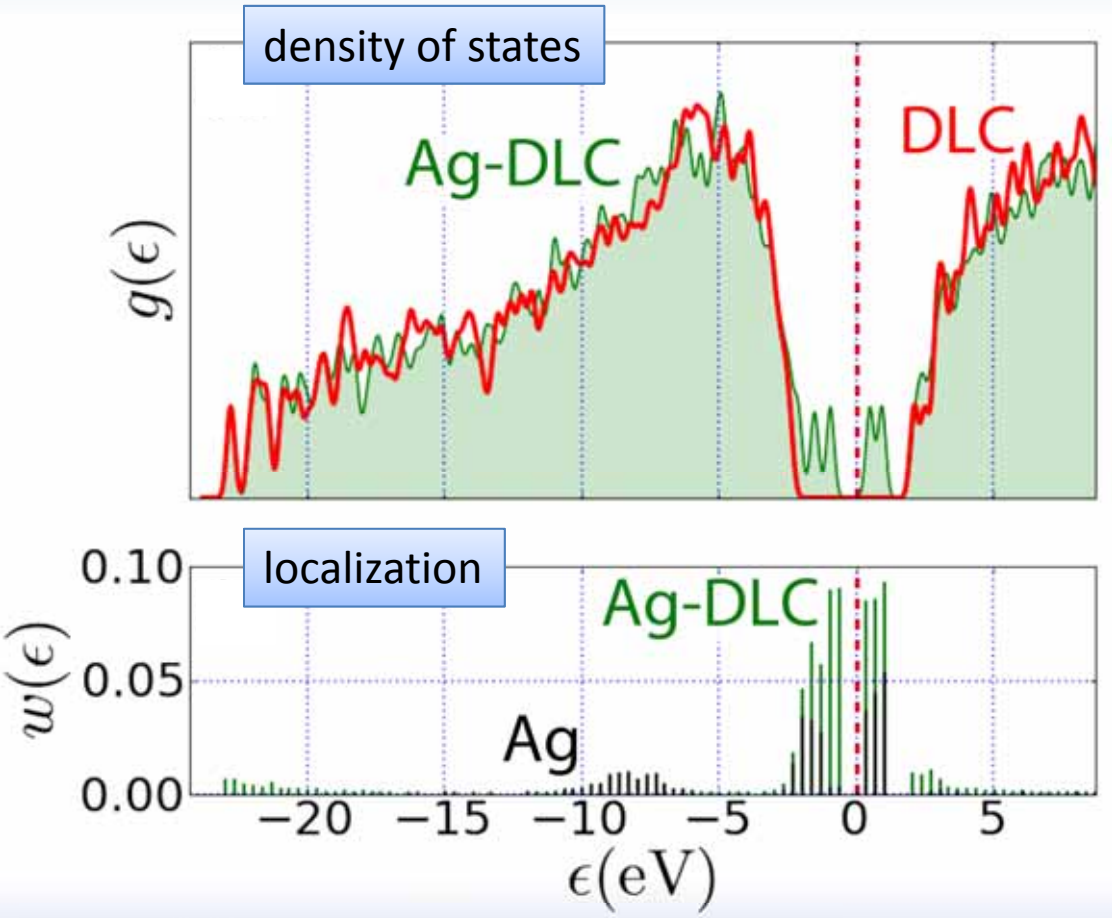



[1] G.M. Matenoglou, H. Zoubos, A. Lotsari, C.E. Lekka, P. Komninou, G.P. Dimitrakopulos, C. Kosmidis, G.A. Evangelakis, and P. Patsalas, Thin Solid Films **518**, 1508 (2009)

# Electronic properties

The metallic inclusions introduce states into the DLC band gap




$w(\epsilon) = \sum (Ng_i(\epsilon)/g(\epsilon) - 1)^2 / N(N-1)$, $g_i$: PDOS on atom "i"

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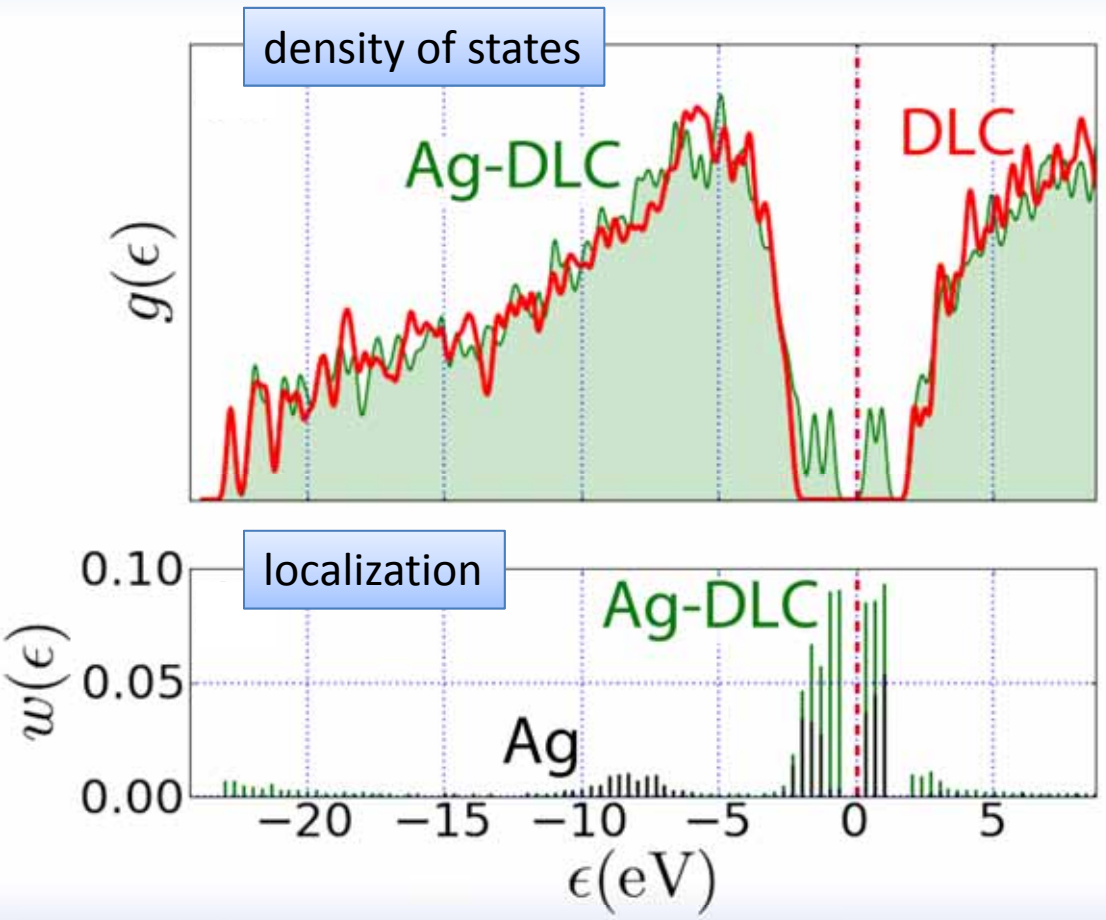
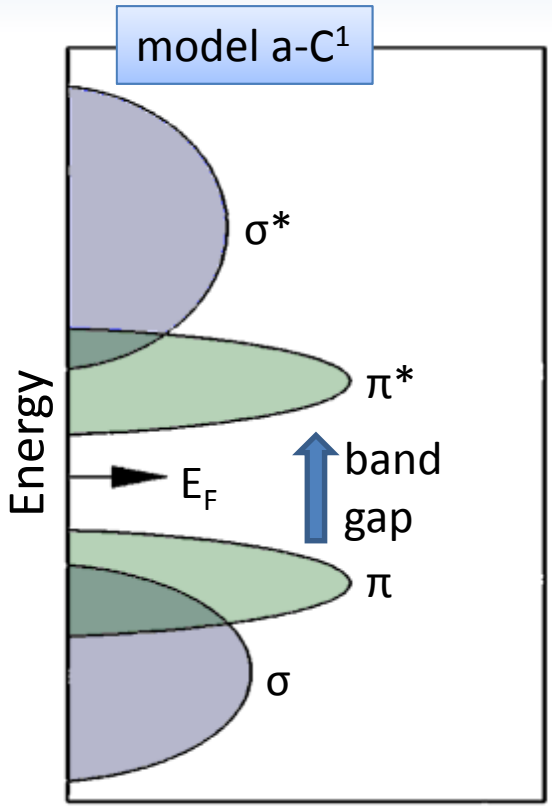


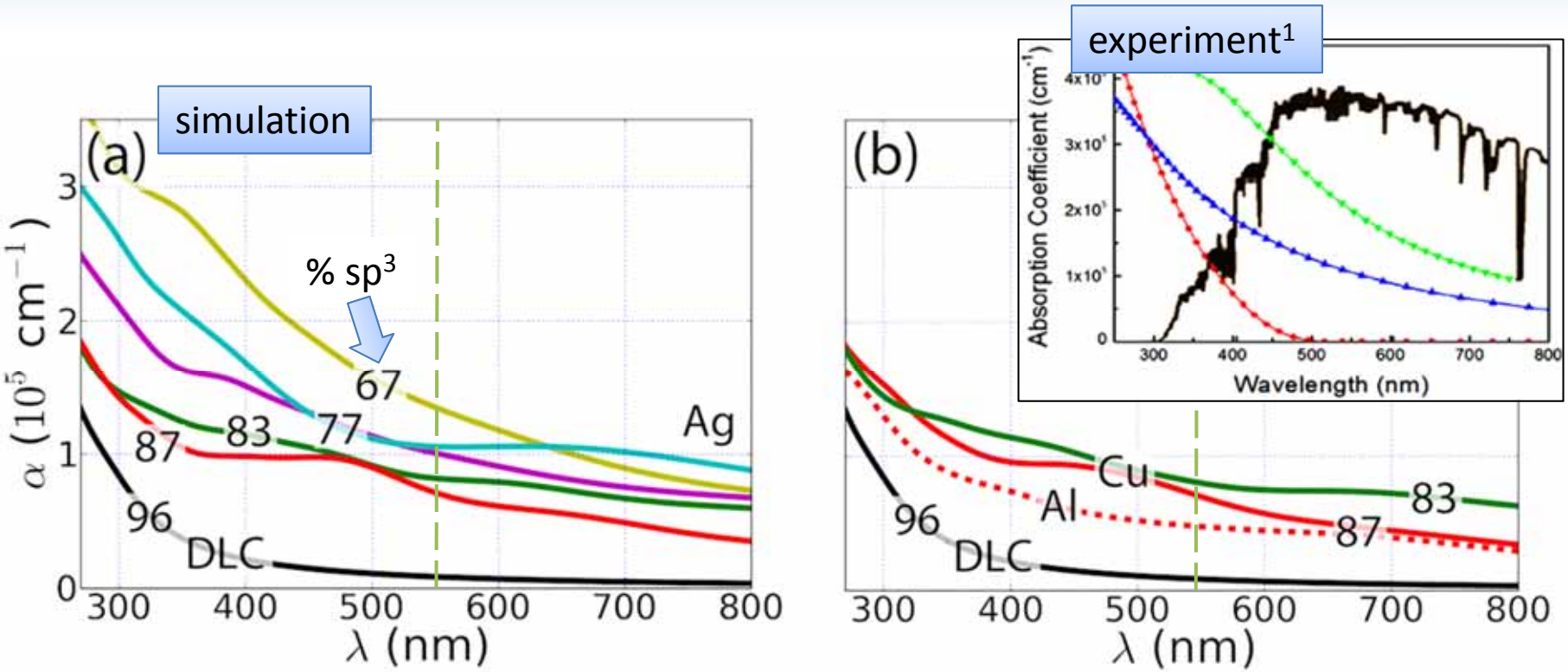




$w(\epsilon) = \sum (N g_i(\epsilon) / g(\epsilon) - 1)^2 / N(N-1)$, $g_i$: PDOS on atom "i"

[1]J. Robertson, Mater. Sci. Eng. R Rep. **37**, 129 (2002).

# Optical properties

## Metal incorporation in DLC enhances absorption in the visible

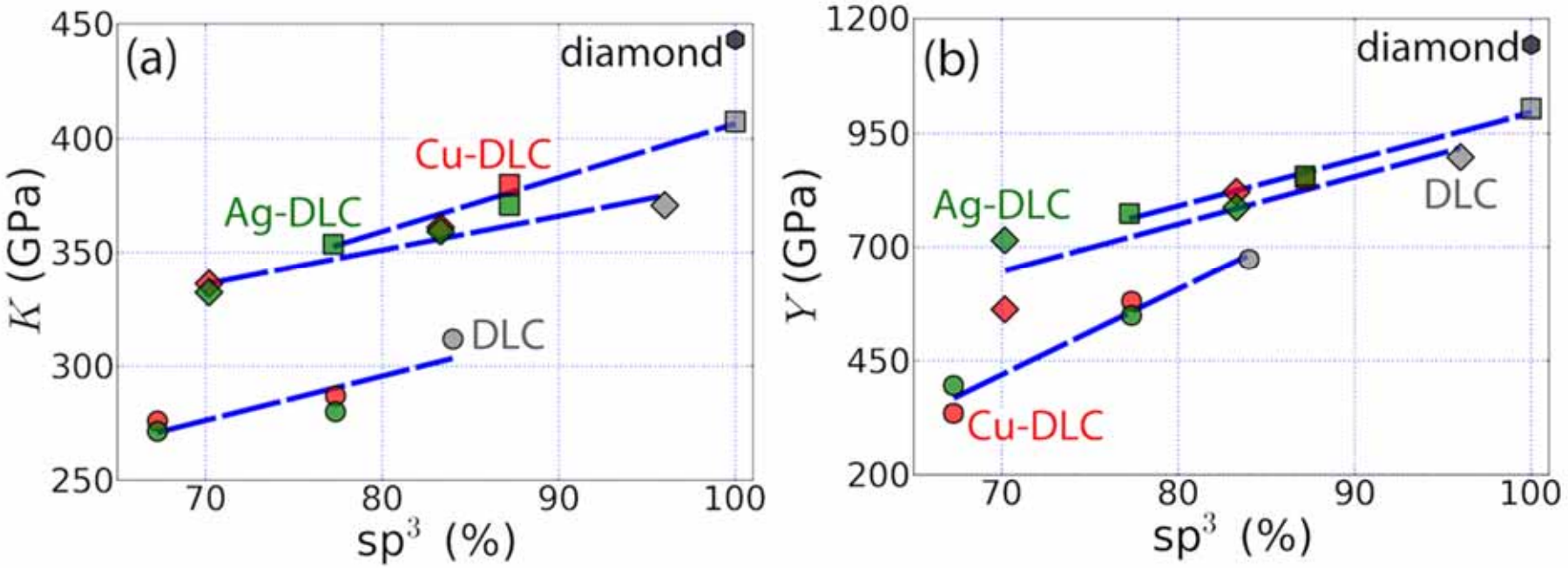



Time-dependent DFT (Bootstrap approximation for the xc kernel[2])

[1]H. Zoubos, G. Constantinidis, D. Pentaras, S. Kalogirou, P.C. Kelires, and P. Patsalas, ICMCTF, San Diego (2011)
[2]S. Sharma, J. K. Dewhurst, A. Sanna, and E. K. U. Gross, Phys. Rev. Lett. 107, 186401 (2011)

# Mechanical properties

Metal incorporation in DLC softens the material



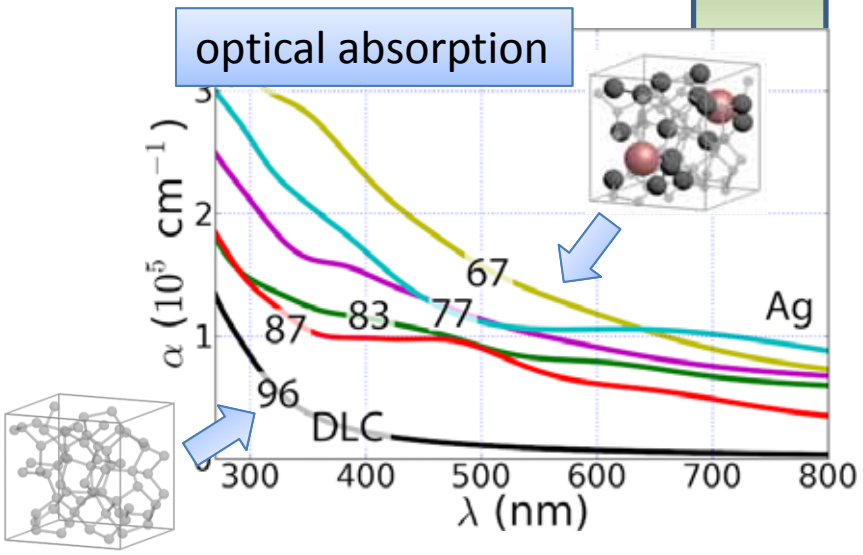

Finite deformation (stress-strain) approach

# Design principles

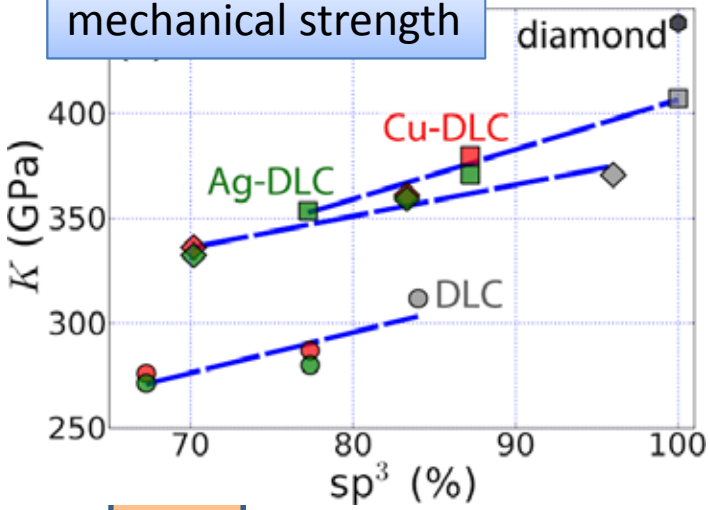
Metal incorporation in DLC enhances absorption in the visible;
The composite softens but retains good mechanical strength

~1.6x10$^3$ cm$^{-1}$ / 5% sp$^2$

optical absorption




mechanical strength




~10 GPa / 5% sp$^3$

# Summary

## Design of metal-containing DLC

DLC with 70-80% $sp^3$-bonded C and < 3% at. metal shows high absorption in the visible ($\alpha > 10^5$ $cm^{-1}$) and good mechanical strength ($K$ > 300 GPa, $Y$ > 500 GPa)

Georgios A. Tritsaris, Christos Mathioudakis, Pantelis C. Kelires, and Efthimios Kaxiras, Submitted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# Thank you, I appreciate your time!

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