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# *Ab initio* Studies of 1-photon and Coherent 2-photon Photoemission on $Cs_3Sb$ and GaAs

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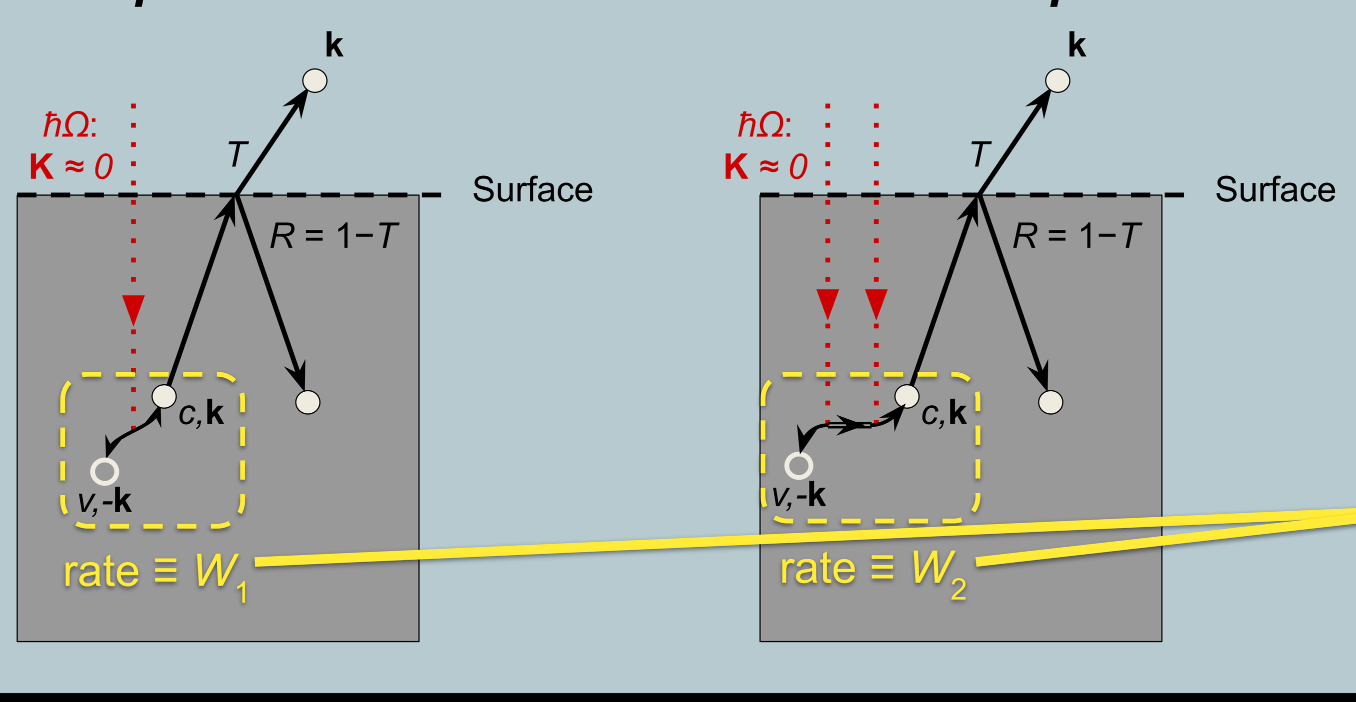
## *Ab initio* Photoemission Calculations

Bulk processes studied since more bulk $e^-$ than surface $e^-$

- Photon(s) excite $e^-$-$h^+$ pair in 2 ways:
  - 1-photon excitation
  - Coherent 2-photon excitation
- Coherent outgoing scattering state
  - $E_\perp > 0 \Rightarrow$ use $T = 100\%$
  - $E_\perp \leq 0 \Rightarrow T = 0$



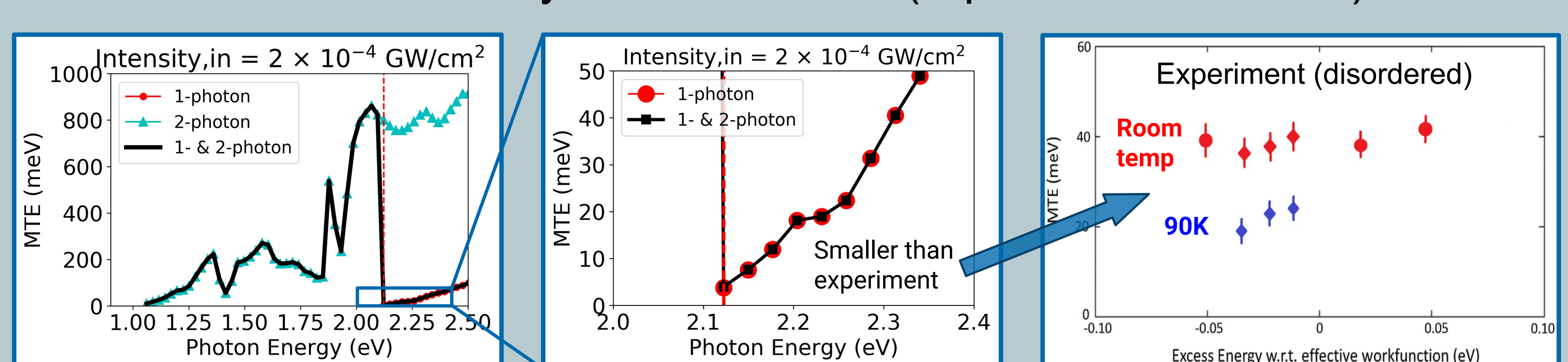

Use ***absorption coefficient α*** to compare numbers of excited electrons

$$\alpha_n = \frac{n\hbar\omega}{I_{\text{in}}} W_n$$

- $n$ = 1 (1-photon) or 2 (coherent 2-photon)
- $I_{\text{in}}$ = laser intensity inside material
- $W_n$ = transition rate of process $n$

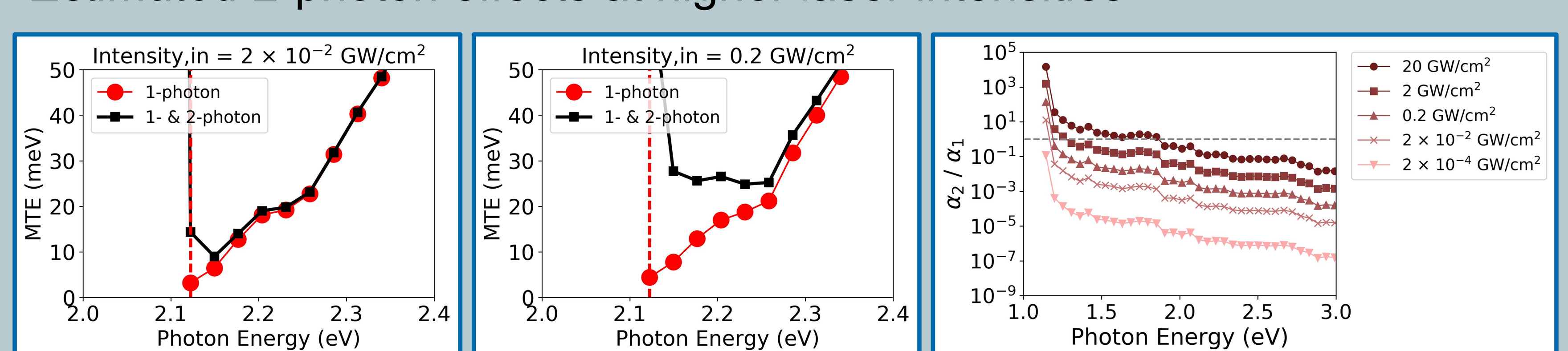
## *Results: Ideal $Cs_3Sb(100)$*

- MTE at low laser intensity inside material (1-photon dominates)




L. Cultrera et al, Phys. Rev. ST Accel. Beams **18**, 113401 (2015).

- *Estimated* 2-photon effects at higher laser intensities

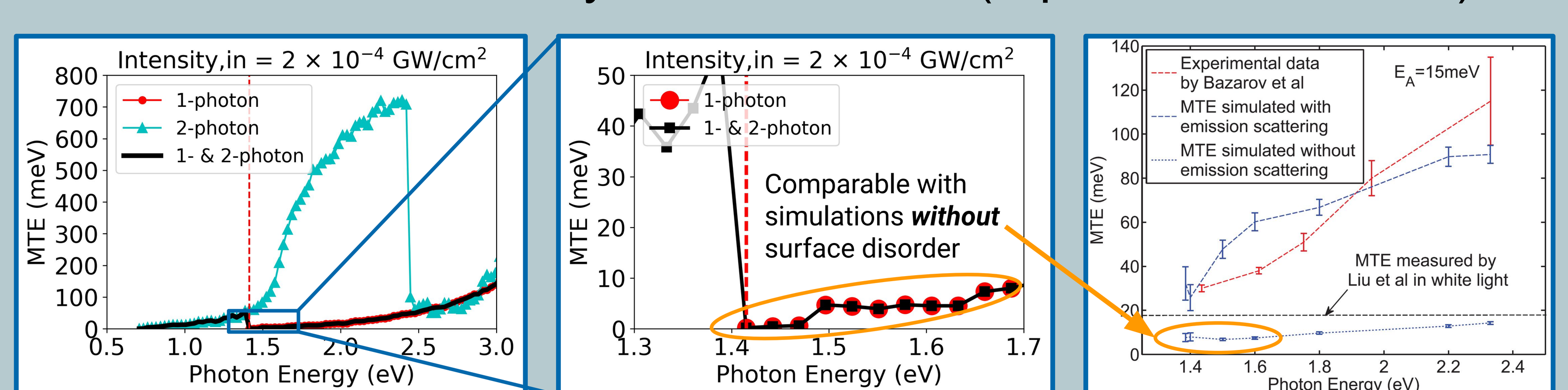



Estimated $W_2$ by scaling Im $\Sigma_{\text{e-phon}}$ to what they should be

- $W_2 \propto 1/\eta$; $\eta \equiv \text{Im}\,\Sigma_{\text{e-e}} + \text{Im}\,\Sigma_{\text{e-phon}} \approx \text{Im}\,\Sigma_{\text{e-phon}}$ (~$10^4$x Im $\Sigma_{\text{e-e}}$)
- Im $\Sigma_{\text{e-phon}}$ too large; see "$Cs_3Sb$ Re-relaxed Structure"

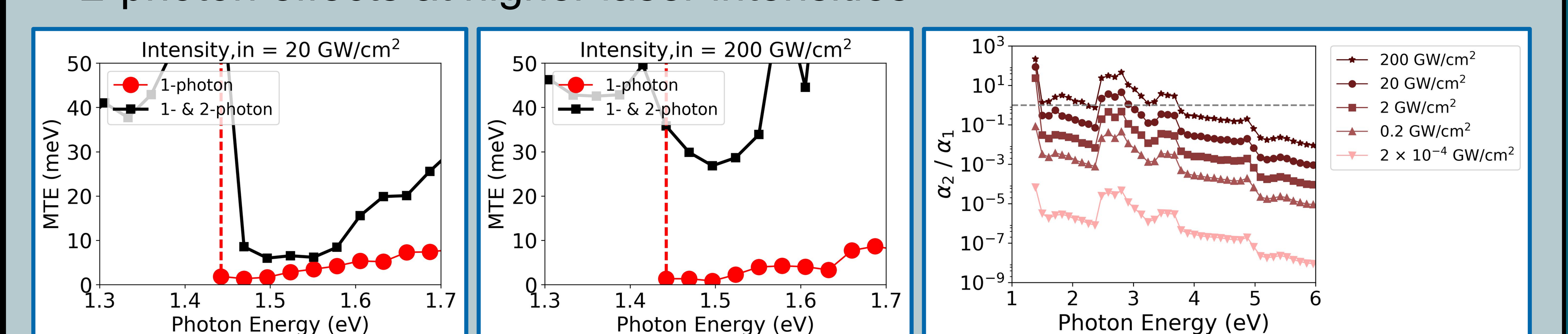
## *Results: Ideal GaAs(100) with $E_A = -0.02$ eV*

- MTE at low laser intensity inside material (1-photon dominates)




S. Karkare *et al.*, erratum to J. Appl. Phys **117**, 109901 (2015).

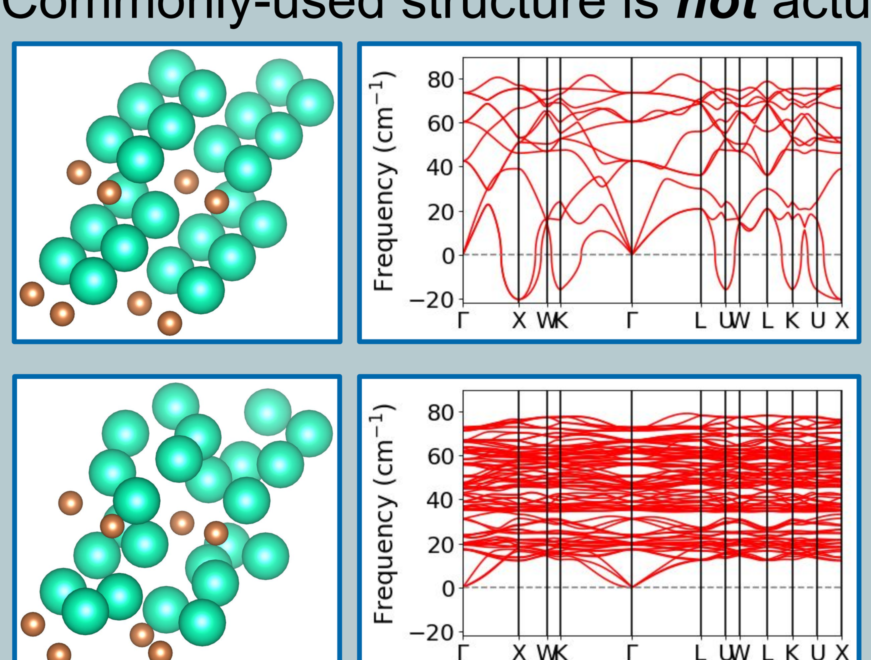
- 2-photon effects at higher laser intensities




- Future work:
  - Integrate to ultrafast-electron-heating Monte Carlo code (see O. Chubenko's and J. K. Bae's posters)

## $Cs_3Sb$ Re-relaxed Structure

- Commonly-used structure is ***not*** actual ground state




Commonly-used structure has *imaginary phonon frequencies*

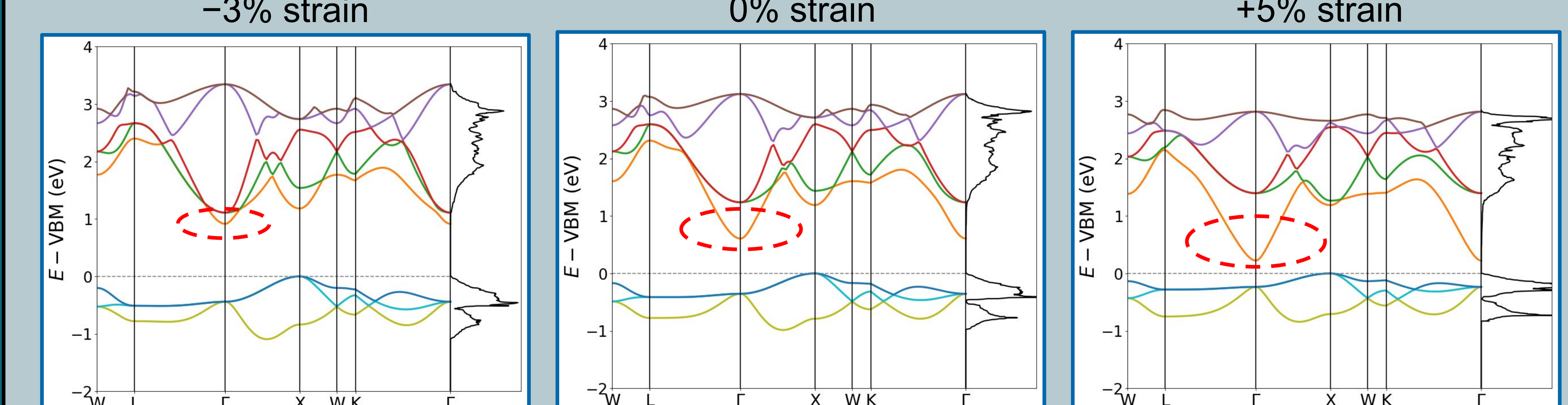
Re-relaxed structure using 2 × 2 × 2 primitive FCC unit cell

- New Im $\Sigma_{\text{e-phon}}$ ~ 0.01x old Im $\Sigma_{\text{e-phon}}$ (~100x Im $\Sigma_{\text{e-e}}$)
- Future work: Re-calculate MTE etc. for $Cs_3Sb(100)$ using this re-relaxed, ***stable*** structure

## "Mid-gap states" in Ideal $Cs_3Sb$

- Preliminary studies show band in gap with very low DOS
  - Energy highly depends on lattice constant / uniform strain

−3% strain | 0% strain | +5% strain




- Future work: effects of oxygen defects* and epitaxial strains
  *XPS measurements suggest prevalence of oxides (W. DeBenedetti and M. A. Hines)

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