# Molecular rationale of graphene-polymer interactions and the effect of solvent on graphene transfer

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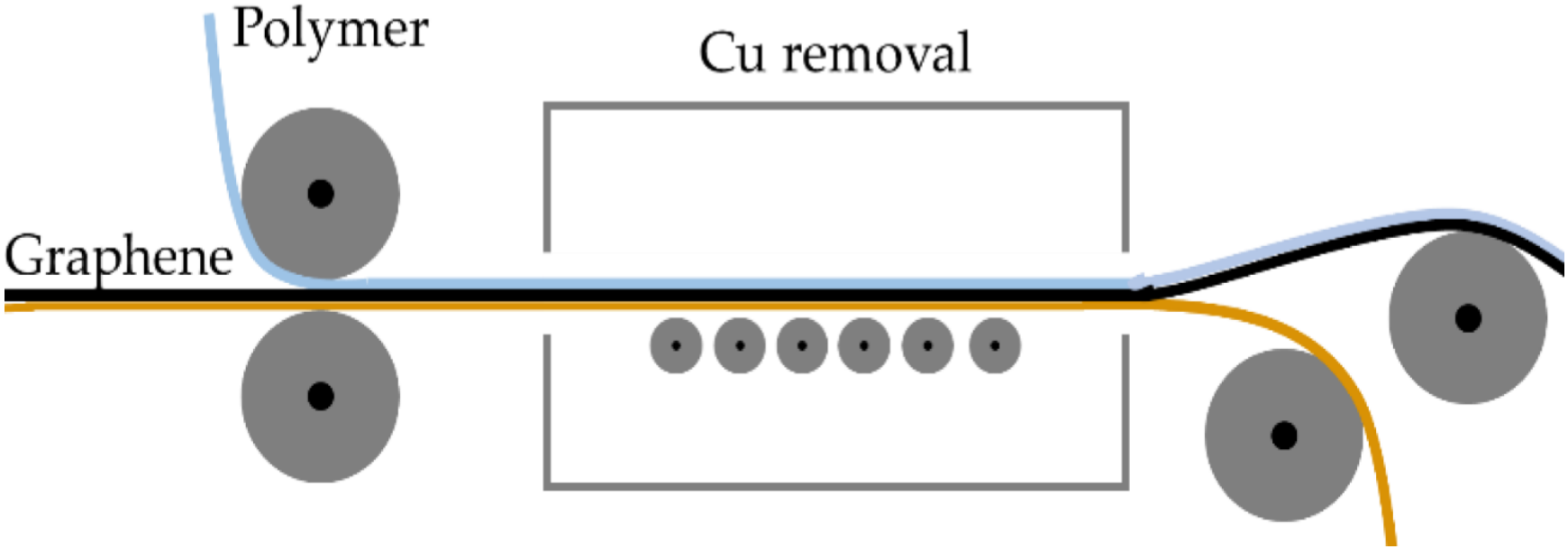
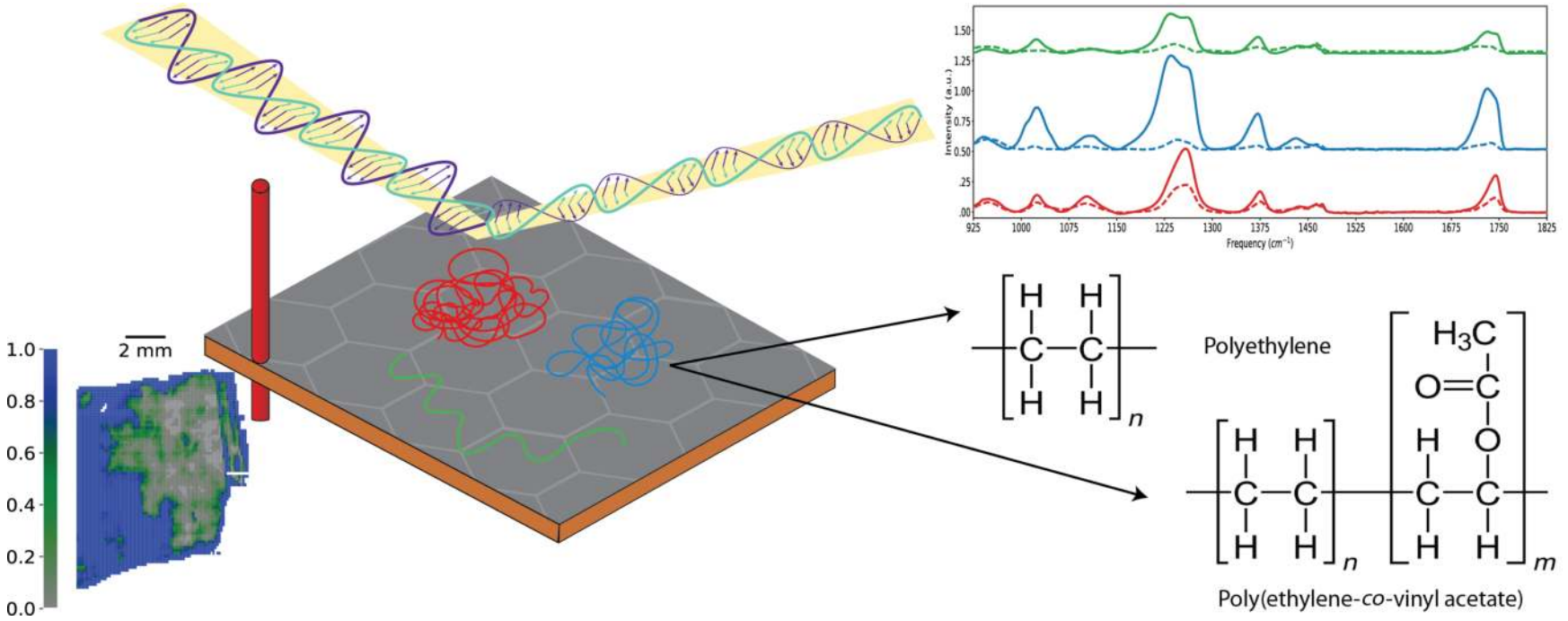
A. J. Carr, A. R. Head, J. A. Boscoboinik, S. R. Bhatia, M. D. Eisaman. Direct evident of graphene-induced molecular reorientation, *Advanced Materials Interfaces,* in review

# Large-scale graphene transfer process for commercialization



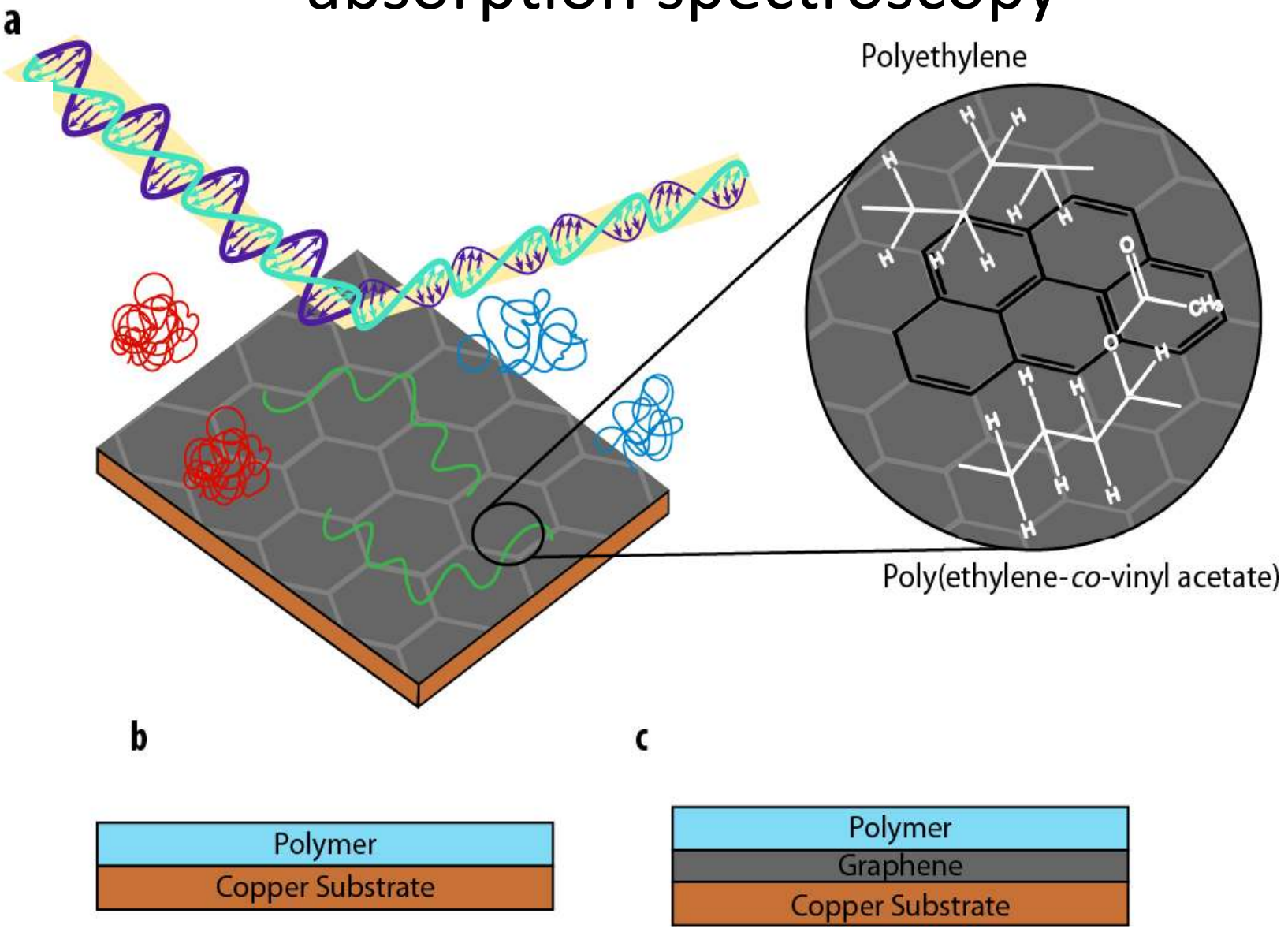

- Successful transfer of graphene from its native copper foil to polymer films is imperative to conductive polymer film development
- Can be integrated into existing roll-to-roll processing

# Graphene-polymer interactions can be tuned via polymer composition and solvent

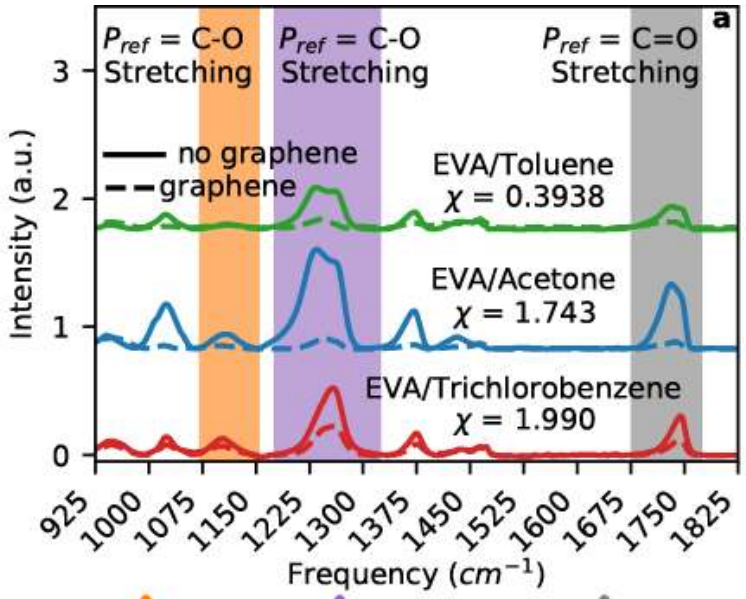


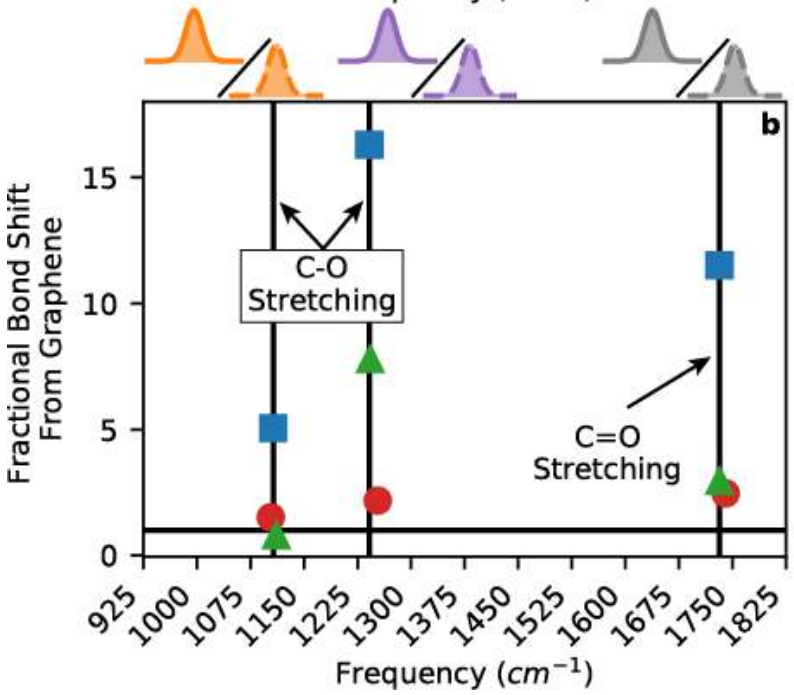

- Both polymer composition and solvent quality impact transfer
- Probe interactions using infrared reflection absorption spectroscopy
- Connect interactions to transfer success across sample area

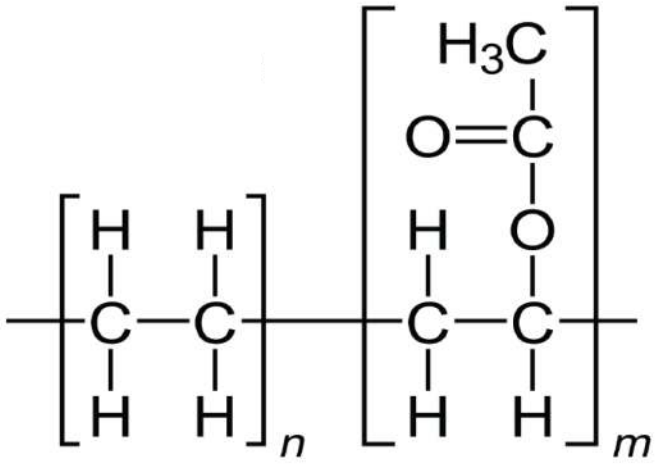
# Probing interactions using Infrared reflection absorption spectroscopy



# Graphene induces polymer rearrangement



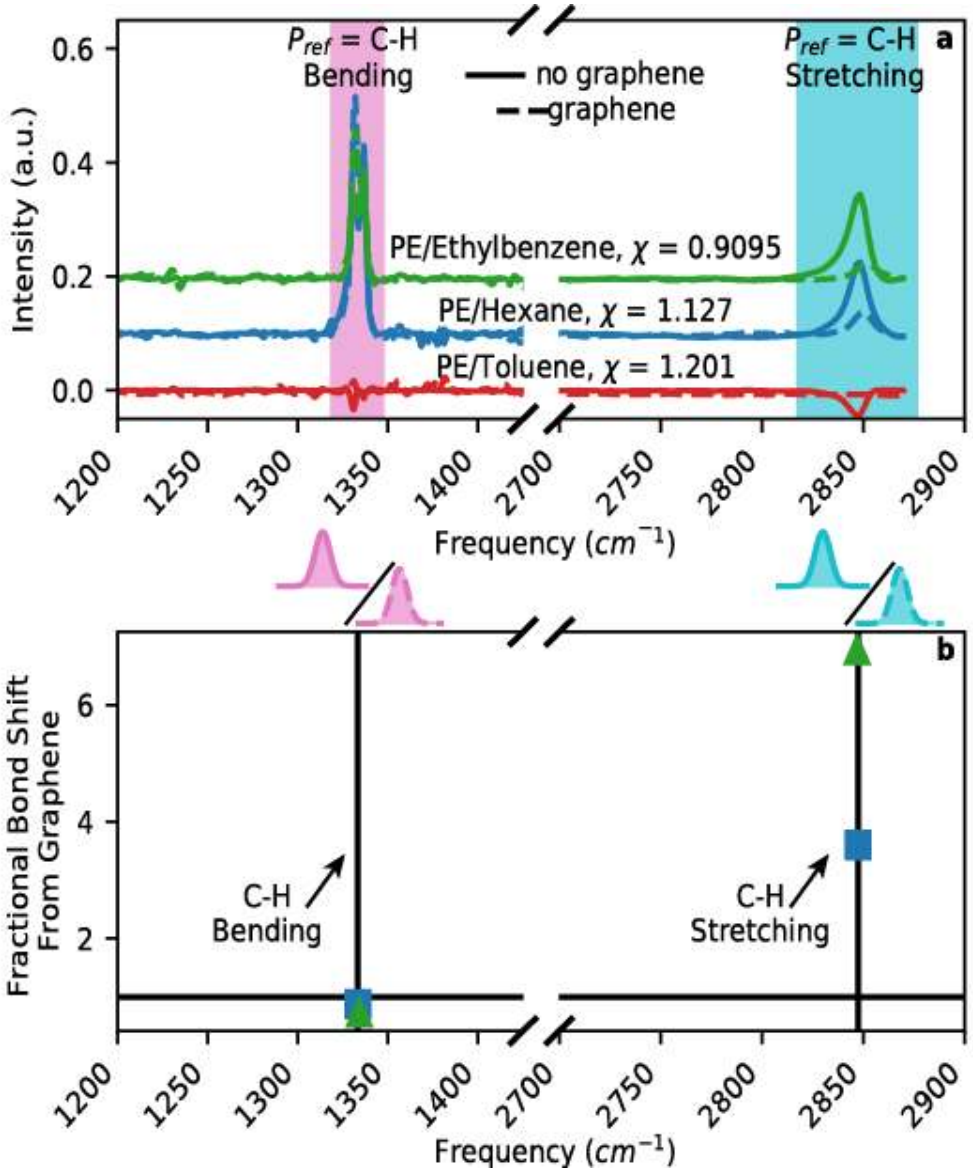



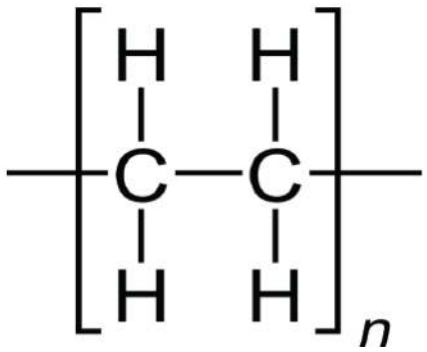




Poly(ethylene-*co*-vinyl acetate)

- In all solvent cases, both C-O and C=O rearrange when we introduce graphene
- Most movement for neutral solvent case; least movement for poor solvent case
- Movement may be linked to favorable molecular orbital overlap

# Graphene induces polymer rearrangement

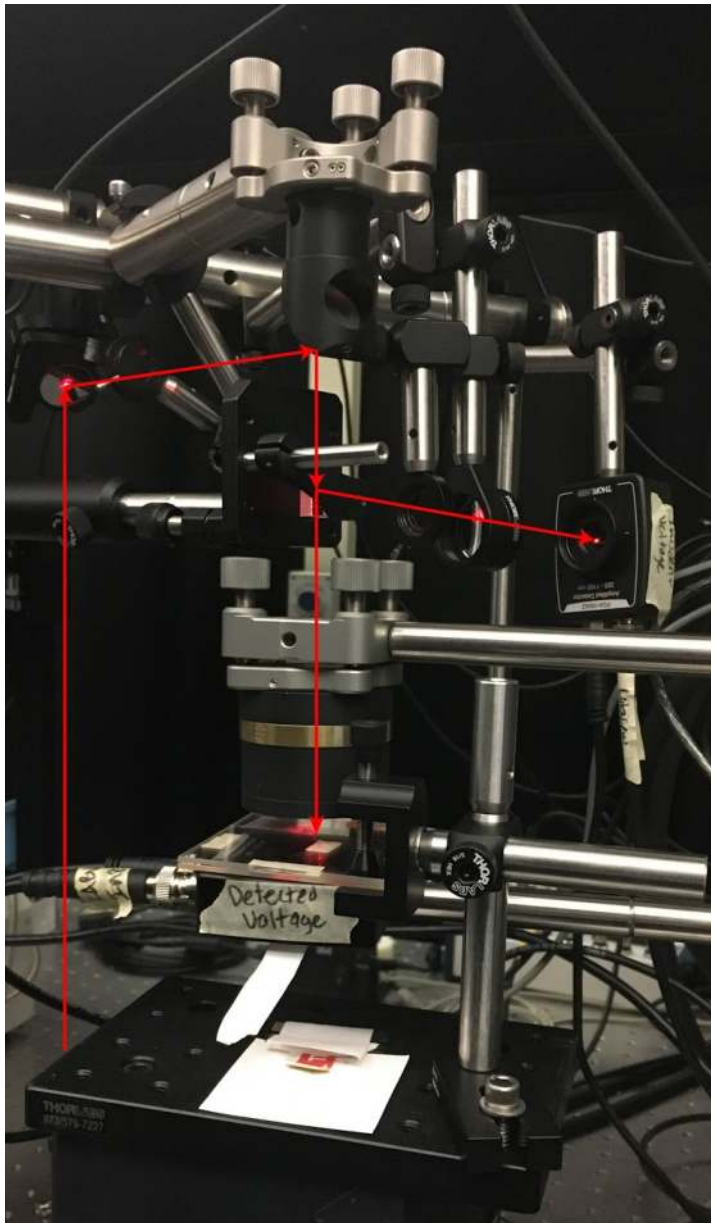


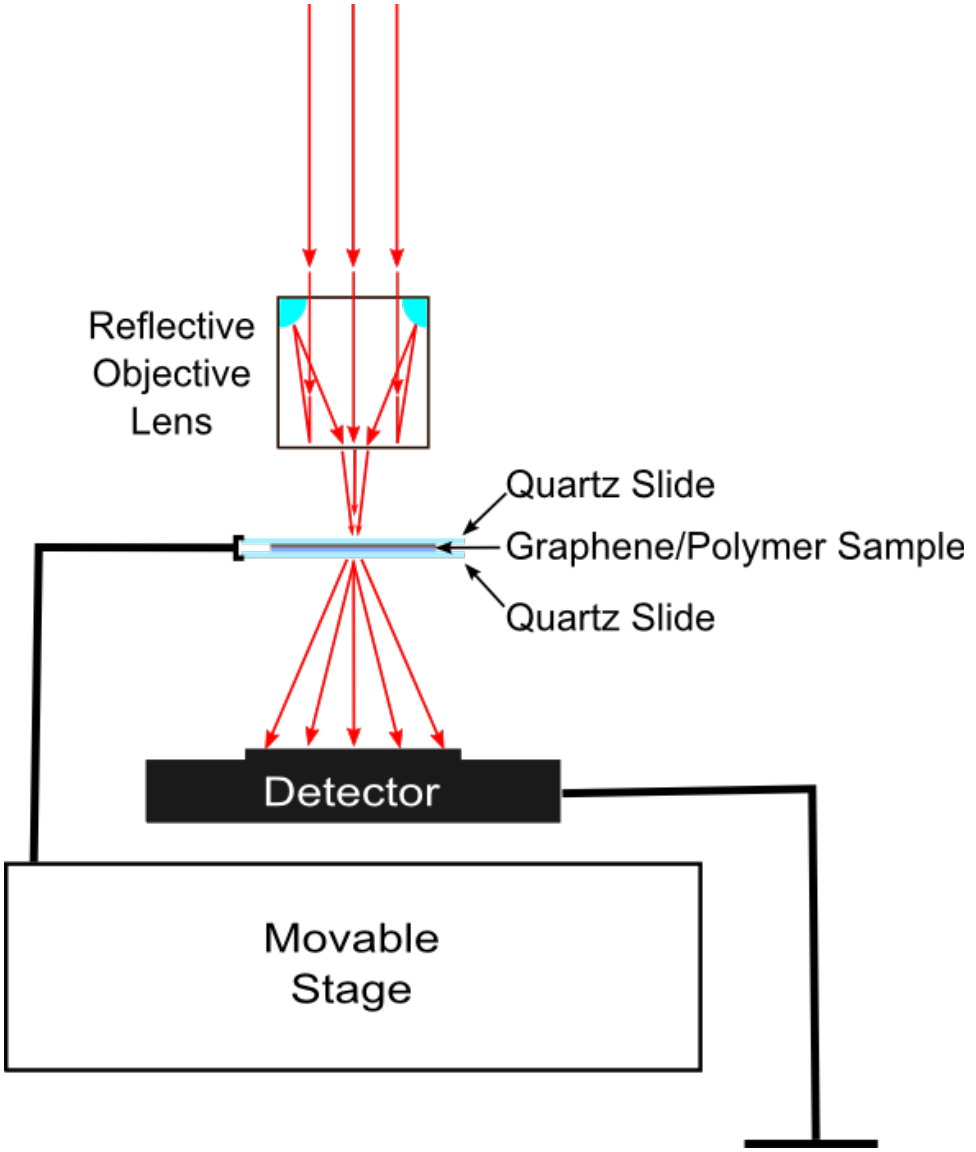




Polyethylene

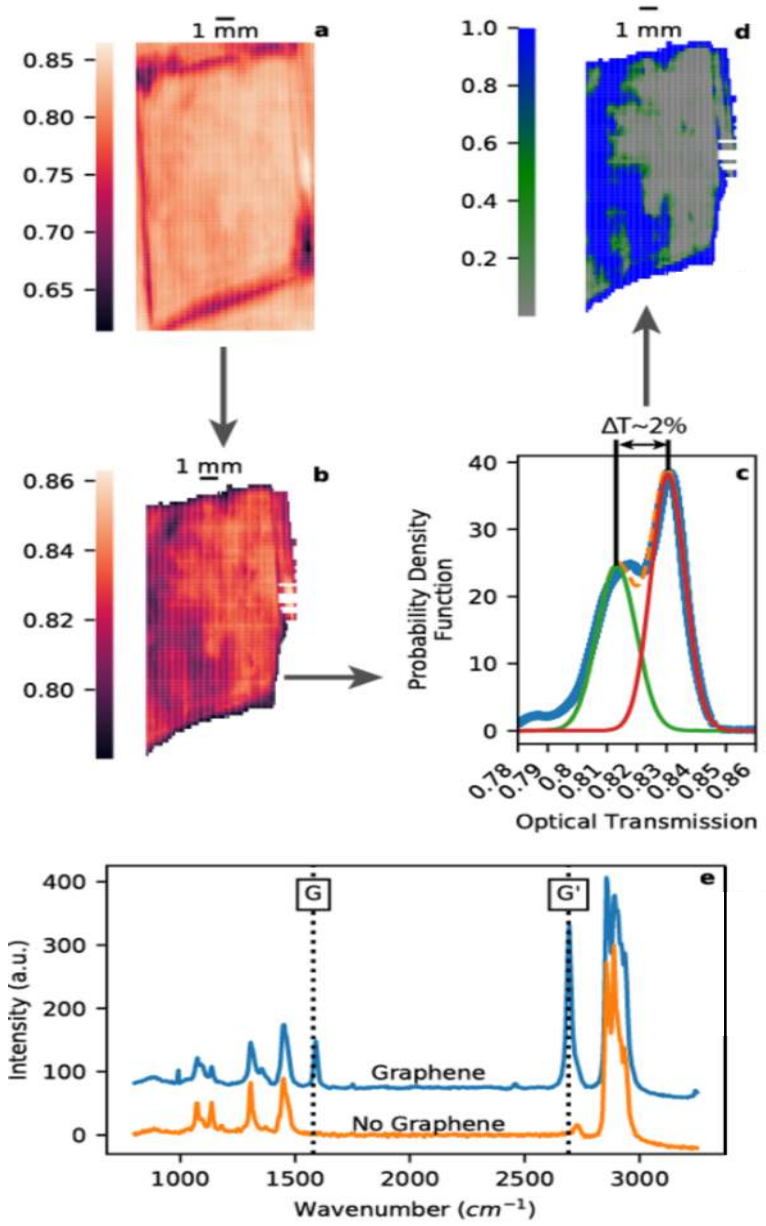
- Poor solvent case shows no polymer chain rearrangement
- Both C-H bending and C-H stretching modes rearrangement when we introduce graphene
- Movement likely linked to unfavorable electronic repulsions

# Optical transmission of graphene/polymer films



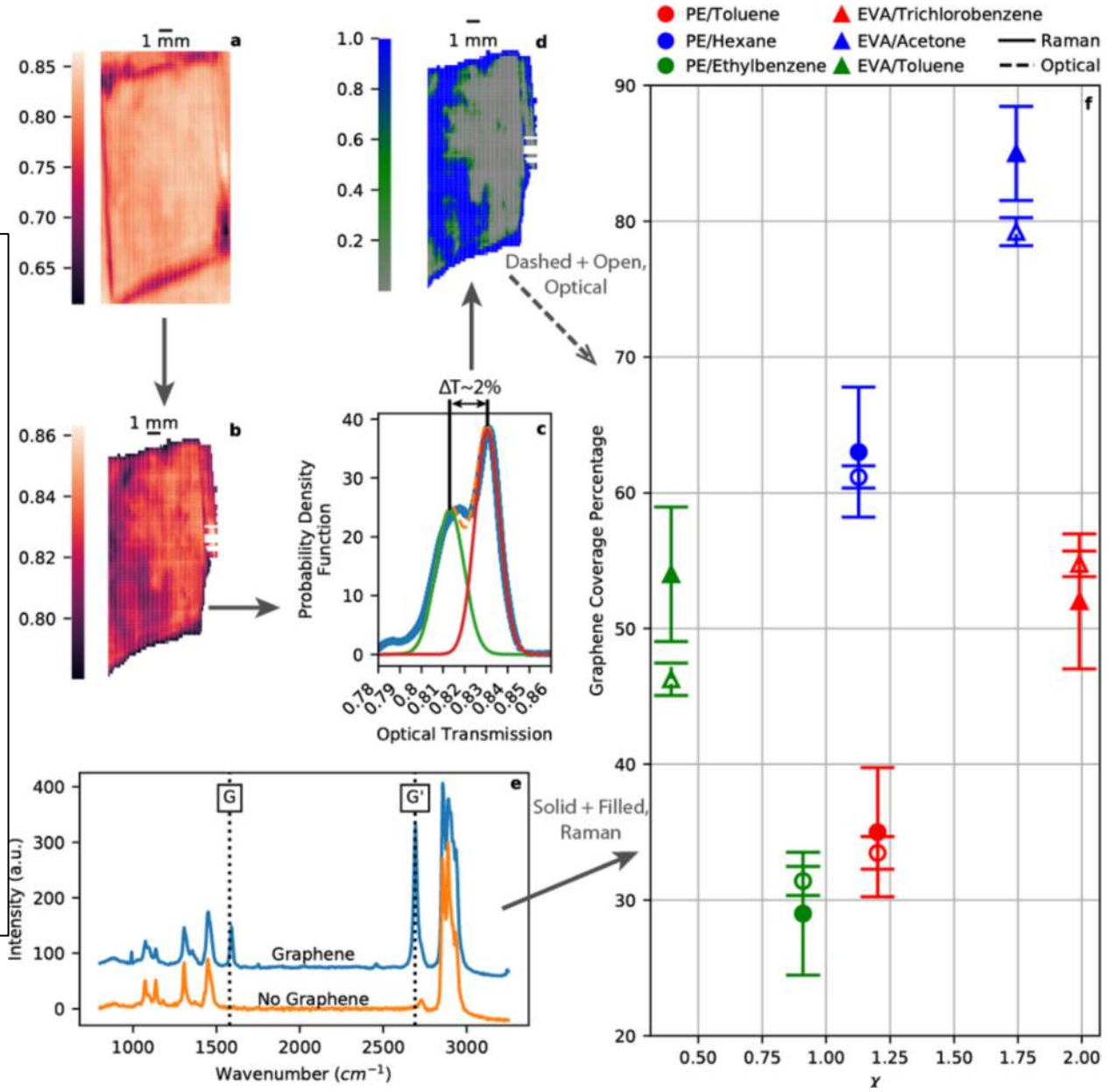
# Quantifying transfer via optical transmission



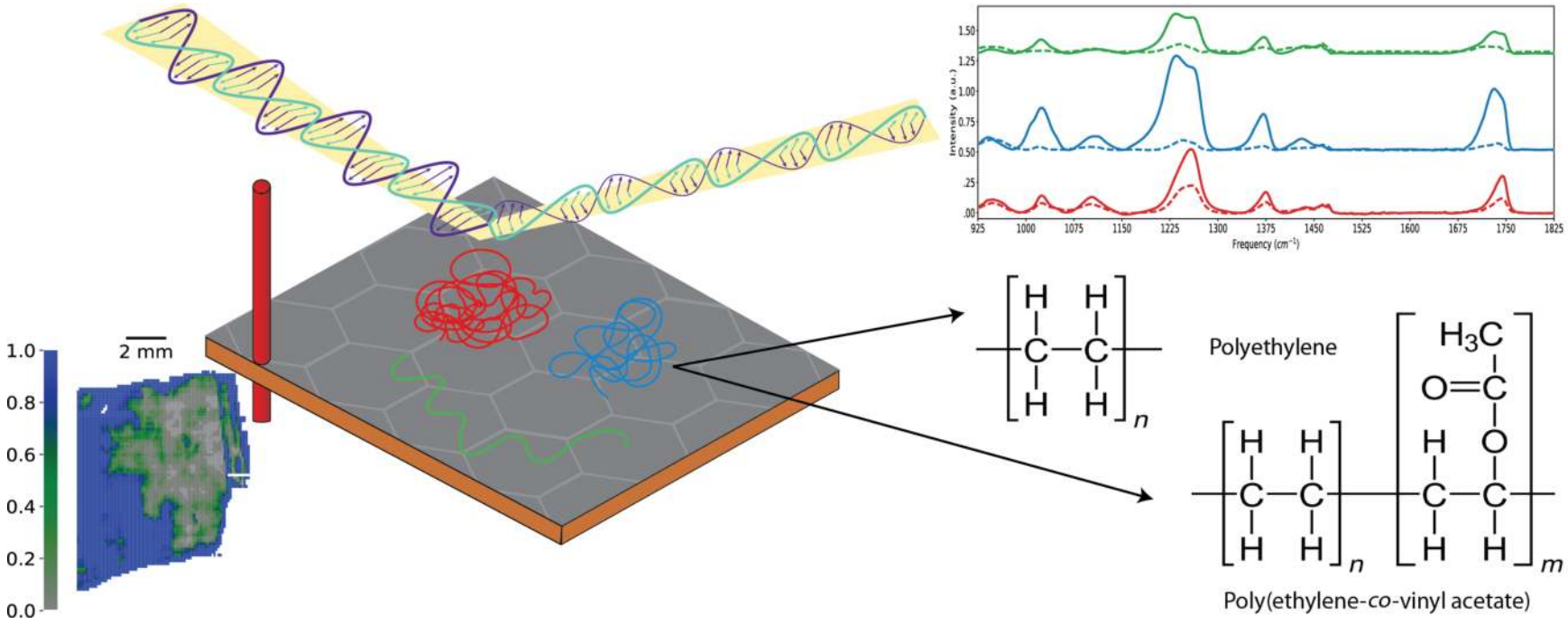

- Optical transmission measured over sample area quantifies transfer success
- Calculate probability of graphene coverage
- We observe
  - 50-85% graphene coverage for poly(ethylene-co-vinyl acetate) samples
  - 30-65% graphene coverage for polyethylene samples

# Neutral solvents and oxygen polymers show best transfer results

- Raman data corroborate optical transmission analysis
- Optimal neutral solvent give best transfer results
- Better transfer to oxygen-containing polymer



# Graphene-polymer interactions can be tuned via polymer composition and solvent




- Graphene transfer success largely depends on polymer chain composition where electronegative moieties are most important
- Solvent choice may affect transfer on a smaller scale

# Acknowledgements

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**Group members:** Joseph Andrade, Jan Folkson, Dr. Mohamed Boukhicha

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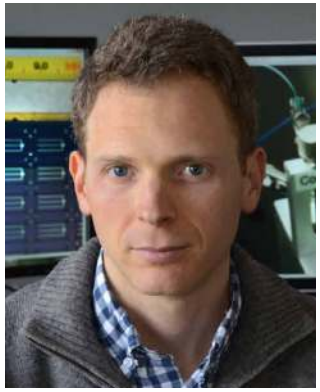


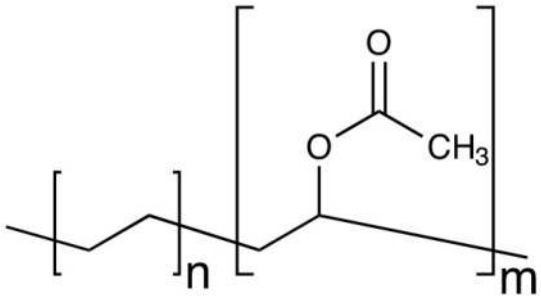



# Experimental Methods

| Polymer | Solvent | Concentration (mg/mL) | χ |
|---|---|---|---|
| Poly(ethylene-co-vinyl Acetate) | 1,2,4-Trichlorobenzene | 10 | 2.0 |
| | Acetone | 40 | 1.7 |
| | Toluene | 30 | 0.39 |
| Polyethylene | Toluene | 40 | 1.2 |
| | Hexane | 30 | 1.1 |
| | Ethylbenzene | 40 | 0.91 |

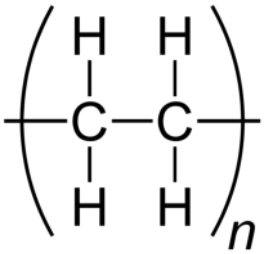
# Applied heat and pressure transfer process

Ethylene vinyl acetate




88% ethylene, 12% vinyl acetate

Polyethylene




Low density, linear