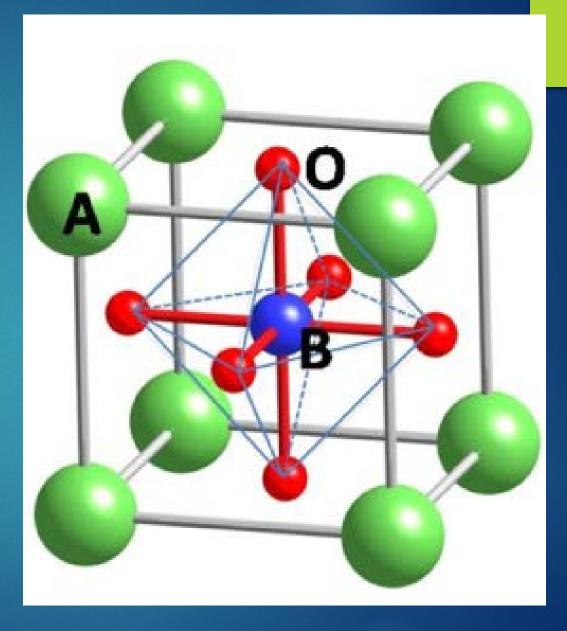
# Visualization of Perovskite Octahedral Tilts in Augmented Reality NAYMAN LEUNG MENTOR - WILLIAM RATCLIFF

# Background

## Perovskites

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- Crystals with ABX<sub>3</sub> structure
  - ► X anion
  - ► A cation
  - ► B cation



Perovskite Unit Cell (Courtesy of Fu and Itoh)

# Crystal Distortions

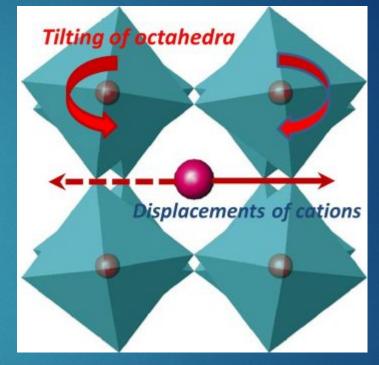
## Distortions

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- Jahn-Teller Distortion
- Cation Displacements
- Octahedral Tilts

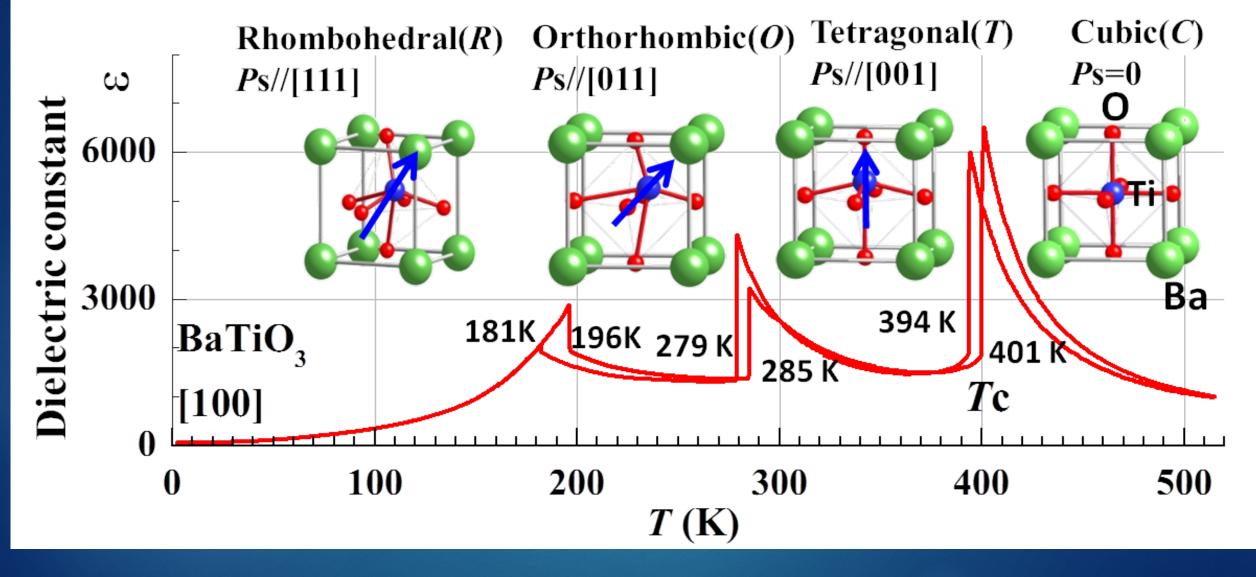
### Causes

- Size of A and B ions
- State Variables



Courtesy of Dr. Gorman





## Cation Size

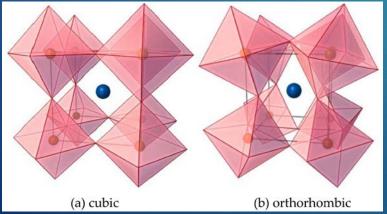
Goldschmidt's tolerance factor (t) - ratio of A and B ionic radii that describe stability

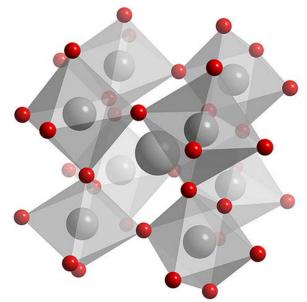
$$t = \frac{r_A + r_0}{\sqrt{2}(r_b + r_0)}$$

>1 = A ion too big or B ion too small = hexagonal

0.9 – 1 = A and B ions are ideal = cubic

0.71 – 0.9 = A ion too small = Orthorhombic/Rhombohedral







Courtesy of Mark Levy

# **Glazer Notation**

Describe octahedral distortion

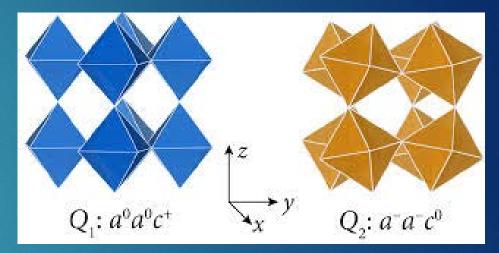
Sequence of symbols – axes

a, a, a – x, y, z

Identical characters – relative magnitude

▶ a, a, c

- Superscript phase of tilt for layers
  - ▶ 0 = no
  - + = in phase
  - = anti phase

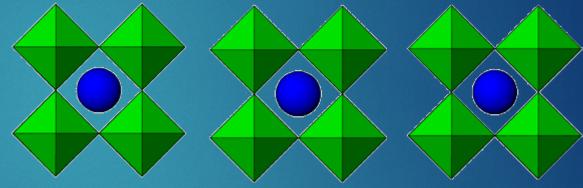


Courtesy of Rondinelli and Fennie

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# Project Goal

- Improve visualization of Perovskite distortions by working in Augmented Reality
- 3D modeling programs
  - VESTA
  - SPuDS
  - Diamond



Courtesy of SPuDS

# Unity3D



Courtesy of Guido Henkel

- Game engine for developing video games
- Language Javascipt/UnityScript, C#, Boo
- Deployment to VR/AR
  - Gear VR (phones)
  - HTC Vive
  - Oculus Rift
  - Windows Hololens



Courtesy of Wired

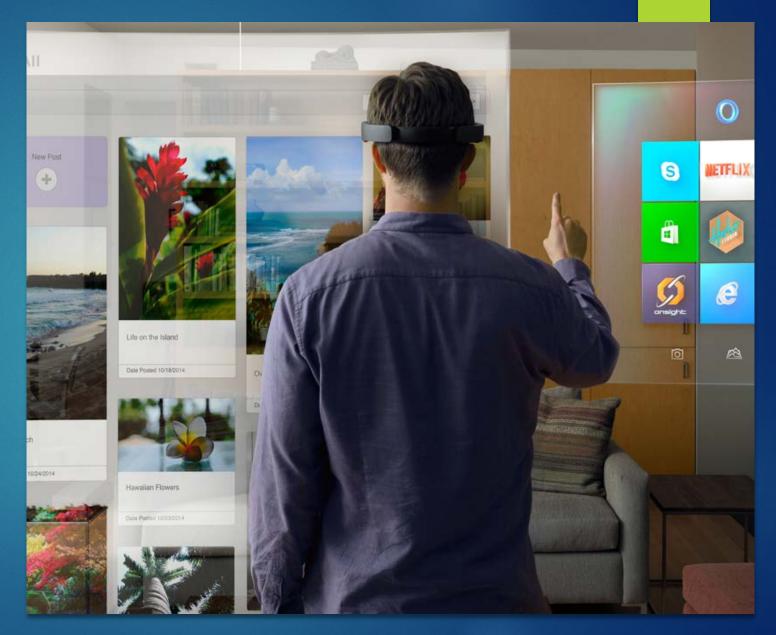


Courtesy of Microsoft



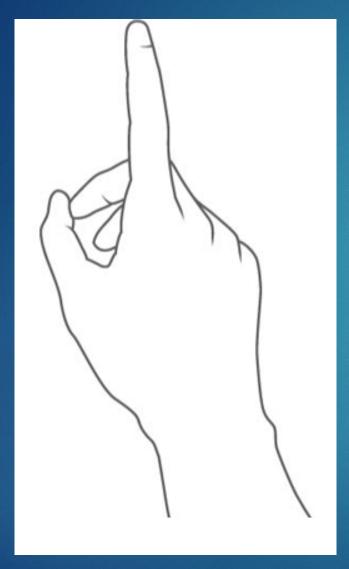
# Microsoft Hololens

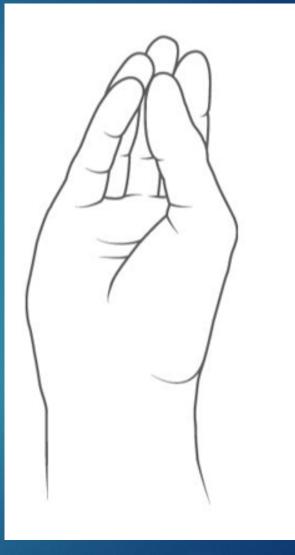
- Augmented Reality
- Spatial mapping, gesture/speech/gaze recognition



Courtesy of Forbes

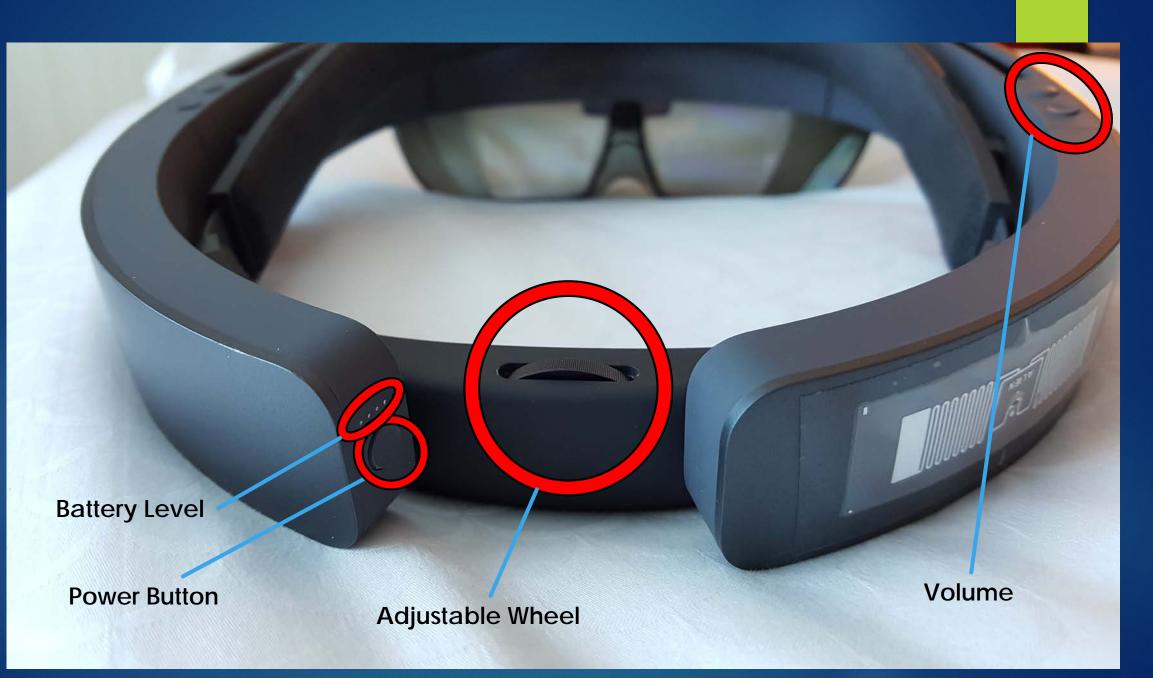












Courtesy of Mark Hachman

# Pin Demo

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Vinity Personal (64bit) - OctahedraTiltModel.unity - OctahedraTiltModel - Windows Store Apps\* <DX11>

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Glazer Stereophotographs	Notation	Unity App Viewed in Hololens
THREE TILTS	a+, b+, c-	
TWO TILTS	a⁰, b⁺, c⁻	
ONE TILT	a <sup>0</sup> , b <sup>0</sup> , c <sup>-</sup>	
NO TILTS	a <sup>0</sup> , b <sup>0</sup> , c <sup>0</sup>	

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# Results

Visualize and manipulate a crystal

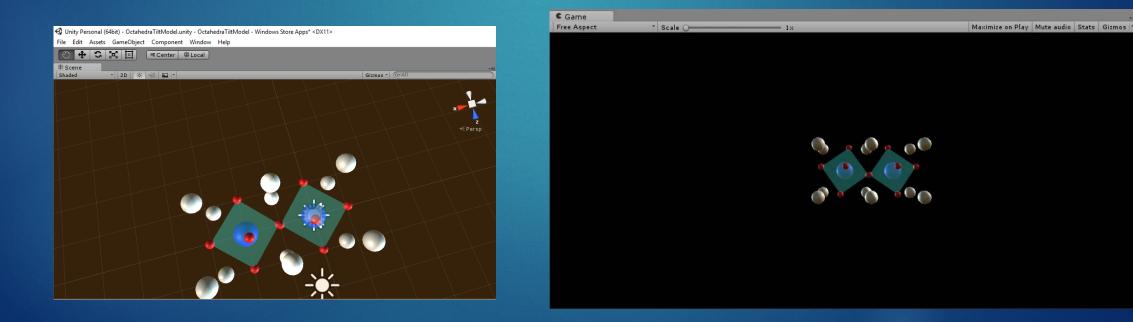
Detect when crystal is being selected (audio)

#### **₽**

# Future Goals

Toolbar – rotation, movement, initiating "octahedral tilt"

- Voice and Spatial Recognition
- Implementation of data



# Practical Applications

## Solar Cells

organic-inorganic semiconductors for efficient photovoltaics

Microelectronics and Telecommunications







Courtesy of Tan, Moghaddam, Lai, et al.

# Acknowledgements

- William Ratcliff
- Don Lopez
- ► NIST, NCNR
- CHRNS

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