# High-throughput identification of defects in SiC

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# Quantum Application

First generation:

- LED
- Laser
- Sensors

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# Quantum Application

Second generation:

- Simulation
- Cryptography
- Computing

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# Specific Applications

## Point defect applications:

- Nano thermometers in cells

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Kucsko, Georg, et al. Nature 500.7460 (2013)

# Specific Applications

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- Nano thermometers in cells
- Chemical sensors, detect 1 part per million

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Aslam, Nabeel, et al. Science 357.6346 (2017)

# Specific Applications

## Point defect applications:

- Nano thermometers in cells
- Chemical sensors, detect 1 part per million
- Photonics, long range entanglement

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Hensen, Bas, et al. Nature 526.7575 (2015)

# Specific Applications

## Point defect applications:

- Nano thermometers in cells
- Chemical sensors, detect 1 part per million
- Photonics, long range entanglement
- and many more...

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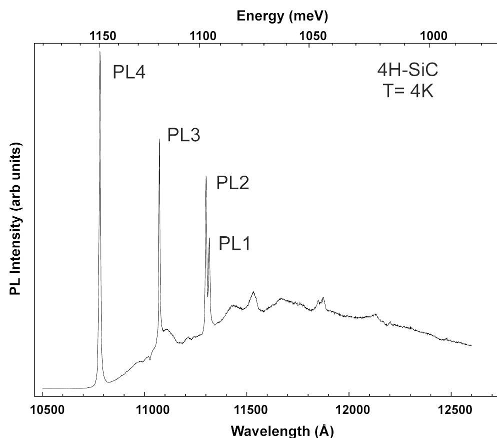
# Photoluminescence to Detect Point Defects

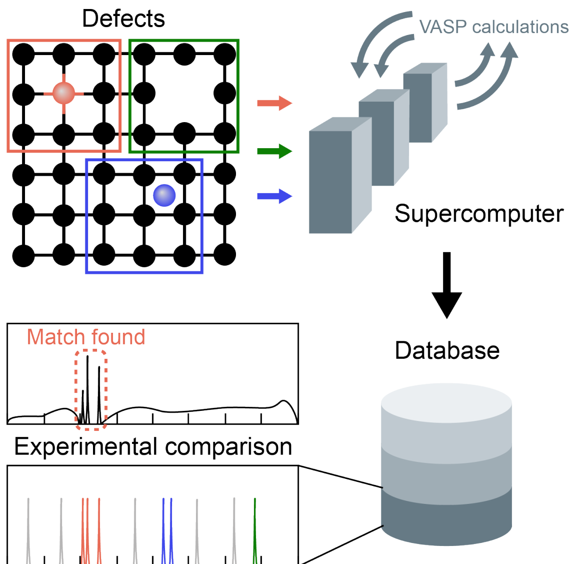



Courtesy of Dr. Ivan Ivanov, LiU

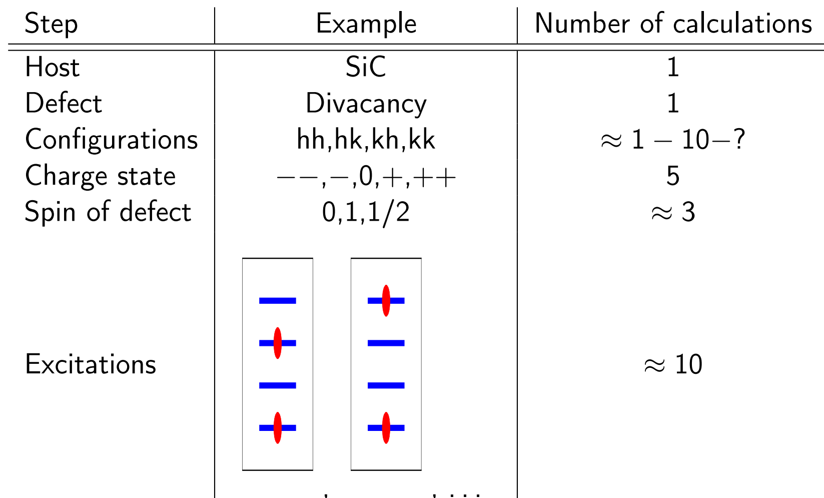
# Movie

The video is available here: `https://d.pr/GKmKFW`

# High-Throughput Search



# Automatic Workflow



| Step | Example | Number of calculations |
|---|---|---|
| Host | SiC | 1 |
| Defect | Divacancy | 1 |
| Configurations | hh,hk,kh,kk | $\approx 1 - 10 - ?$ |
| Charge state | $--,-,0,+,++$ | 5 |
| Spin of defect | 0,1,1/2 | $\approx 3$ |
| Excitations | , , ... | $\approx 10$ |

# Automatic Workflow

To fully characterize one defect in one host material would take about 500 calculations.

With PBE each run would take approximately 800 core-hours.

Total of 400 000 core-hours per defect.

# Results

Stored in database.

Demonstration of prototype web interface.

# Conclusion

- Point defects are useful in a wide range of applications.
- A huge task to find new and interesting point defects.
- Big challenge to match the experimental results with the calculated data in the database.

Thanks to Viktor Ivády, Rickard Armiento, and Igor Abrikosov.