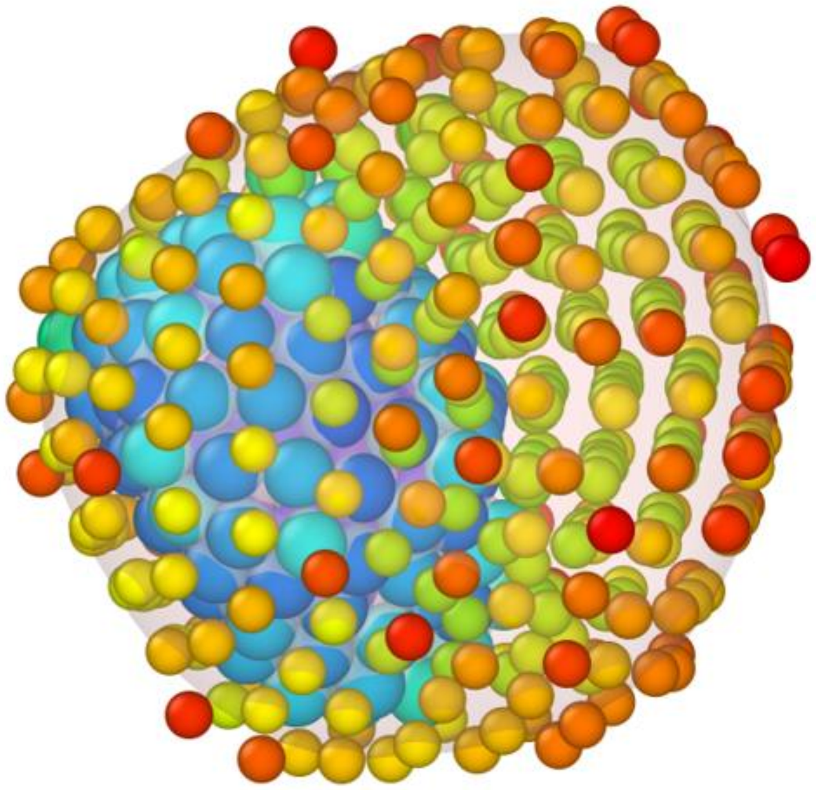


Université d'ORLÉANS

ICMN
Interfaces, Confinement, Matériaux et Nanostructures

Analysis of high-resolution transmission electron microscopy images by deep learning:

Example of AgCo nanoalloys

Daniel Förster

GDR IAMAT 31 May 2022

Convolutional neural networks for HRTEM analysis

Image classification, regression, or denoising

requires large number of examples with known categories, values, perfect images

Proc. of the IEEE **86**, 2278 (1998)

Nanosystems

realistic large-scale data thanks to simulations

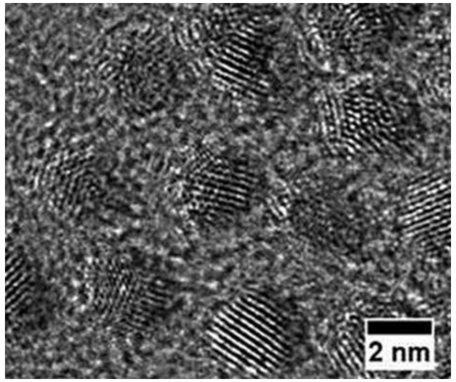
inverse problems: structure determination from experimental characterization techniques

machine learning can add value: reduction of search space when informed by physical models

Advantages: fast, enables thus statistical analysis

Disadvantages: limited scope of applicability, requires validation

Why nanoalloys, why HRTEM?



PdPt nanoalloy

Faraday Discuss., **181**, 19 (2015)

Nanoalloys

- catalysis
- plasmonics
- magnetic particles for biomedical applications

Advantages

- new properties due to alloy effect
- reduced cost
- encapsulation of toxic elements

HRTEM

- analysis of individual objects
- atomic resolution

Difficulties

- image noise, long exposure may affect objects
- aberrations, defocus, Z-insensitivity

Dataset generation: Molecular dynamics

Interatomic model

Tight-binding second moment approximation for Ag-Co

J. Comput. Theor. Nanosci. **6**, 841 (2009)

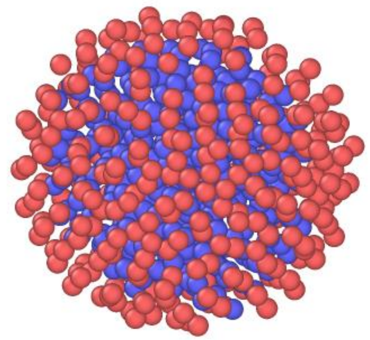
Random system size (up to 1000 atoms), and composition

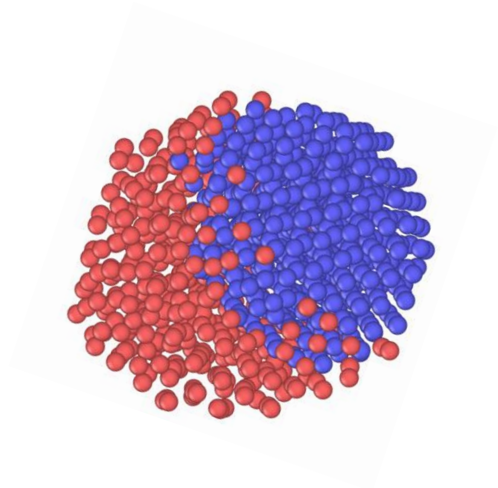
Rapid quench

- **Core-shell:** gas mixture 7500 K to 300 K
- **Janus:** droplets 800 K to 300 K

Thermalization at 300K

200.000 simulations, side effect: enables statistical analysis





Dataset generation: HRTEM images

Multi-slice technique

several software packages available, here Dr. Probe

Ultramicroscopy **193**, 1 (2018)

200 keV electrons, 20 slices

resolution: ~23 px/nm

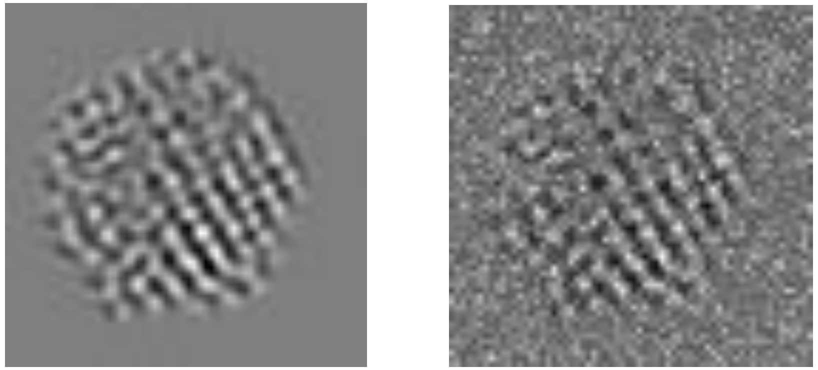
Variability

- random *defocus* and aberration coefficients
- random position and orientation
- addition of shot noise

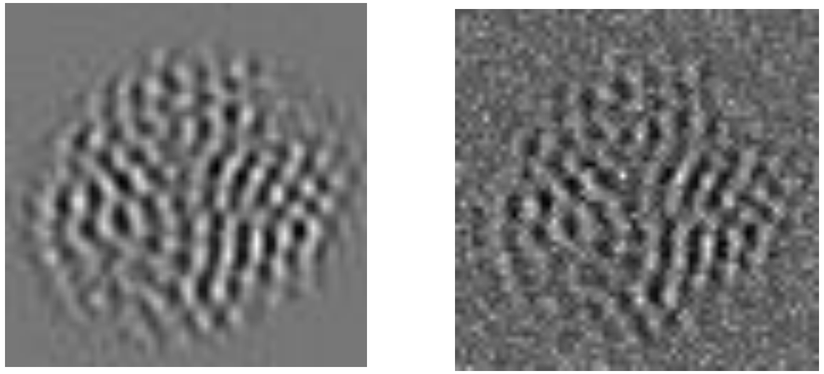
5 images per configuration ➔ 2M images

➔ **realism and diversity are key**

Pairs of clean and noisy images



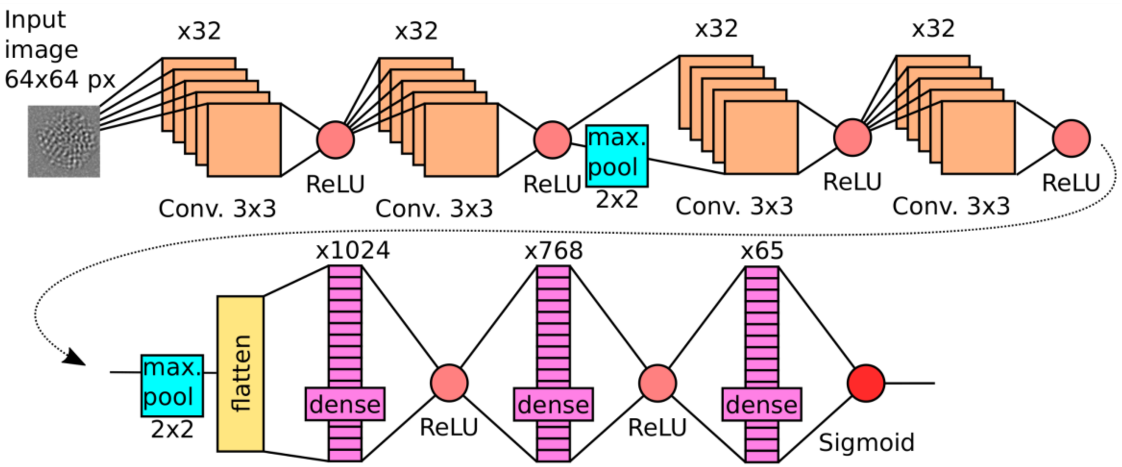
Core-shell



Janus

Classification in terms of chemical ordering

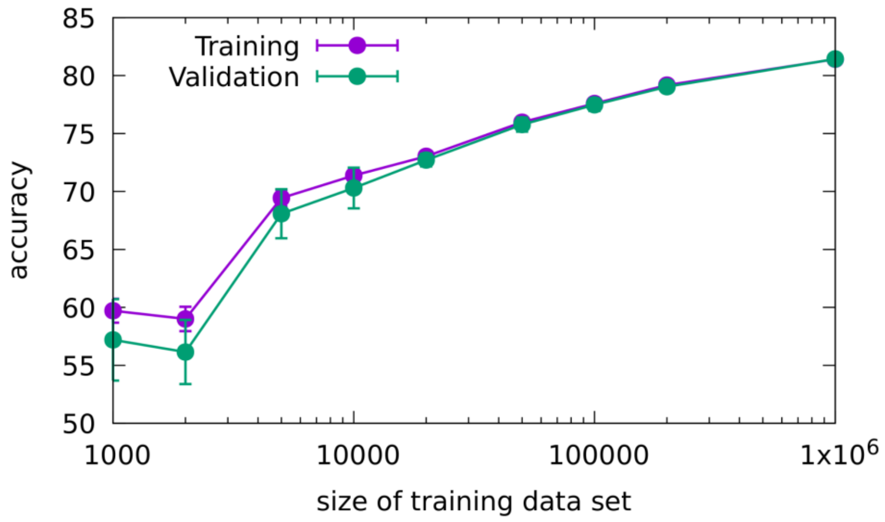
Network architecture



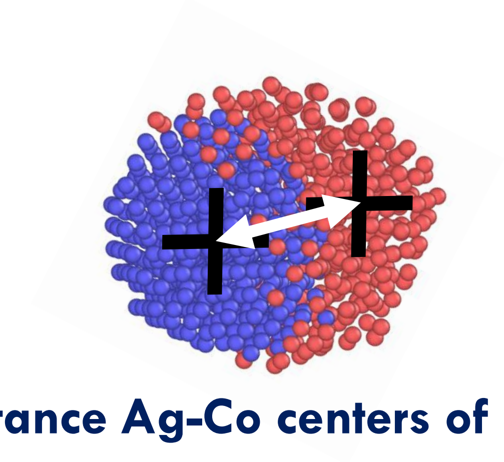
Output value

- **class:** core-shell or Janus
- **size:** number of atoms
- **composition:** N_{Ag}/N_{tot}

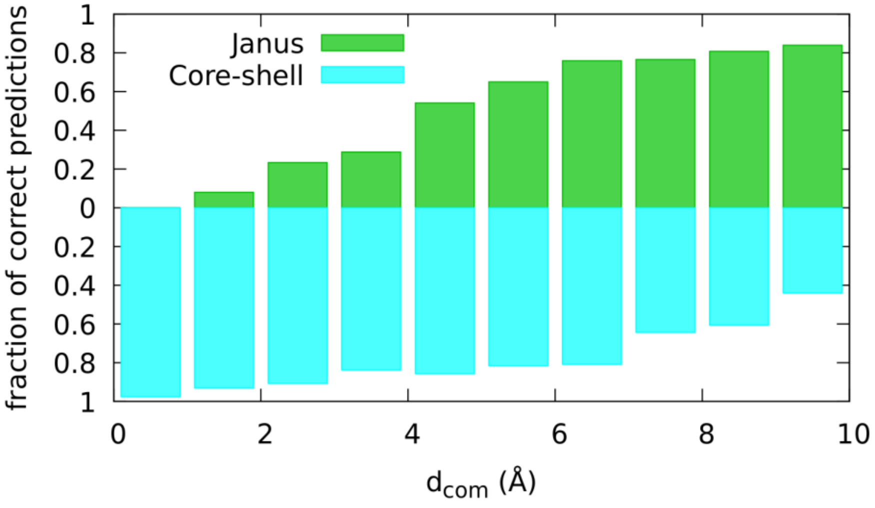
Influence of dataset size



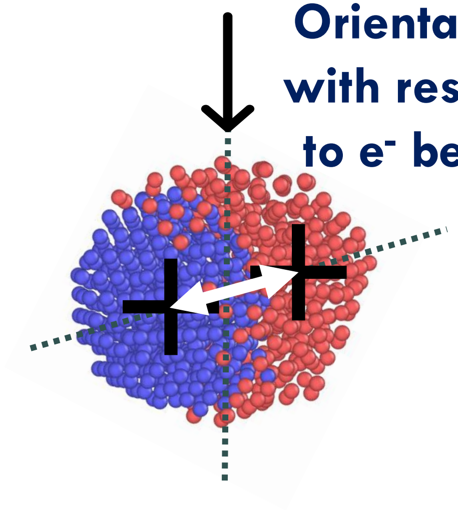
Evaluation of classification accuracy

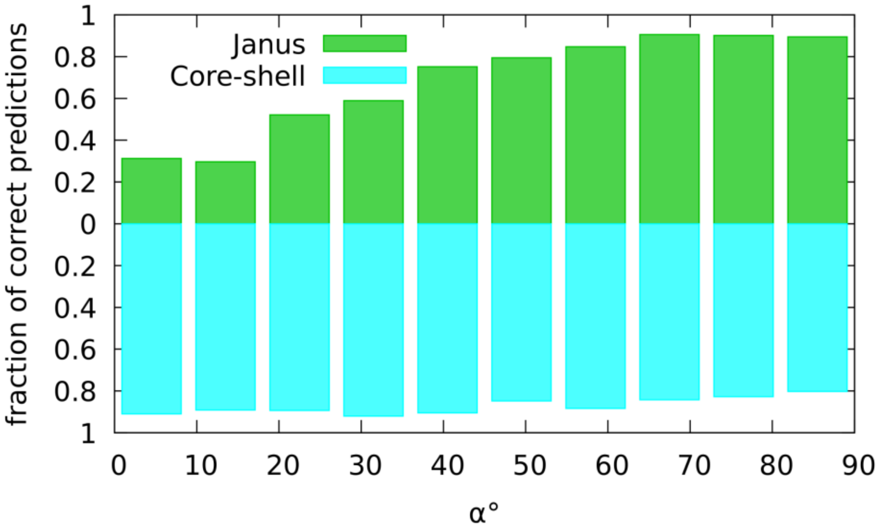


Distance Ag-Co centers of mass



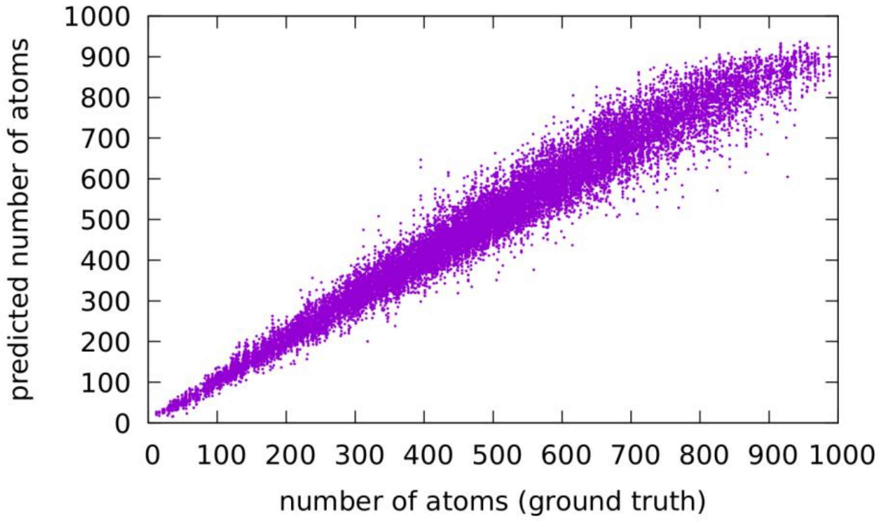
Orientation with respect to e⁻ beam





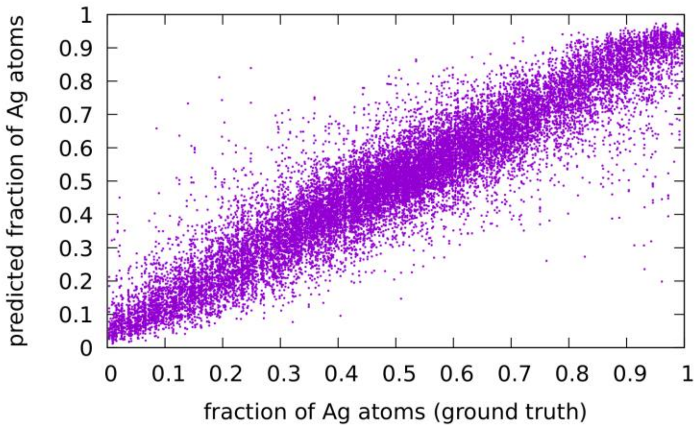
Estimation of particle size and composition

Number of atoms



Average error: ±33 atoms

Particle composition



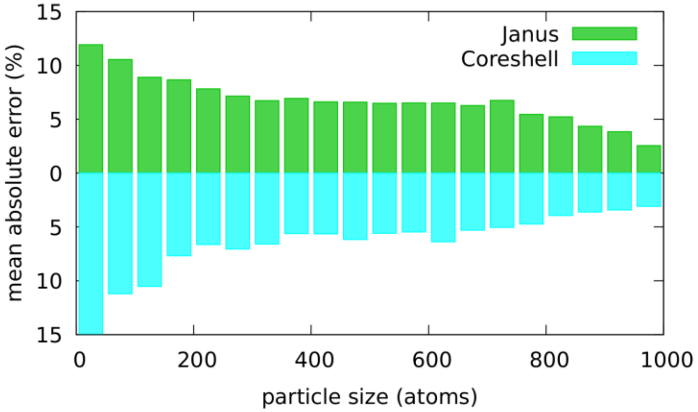
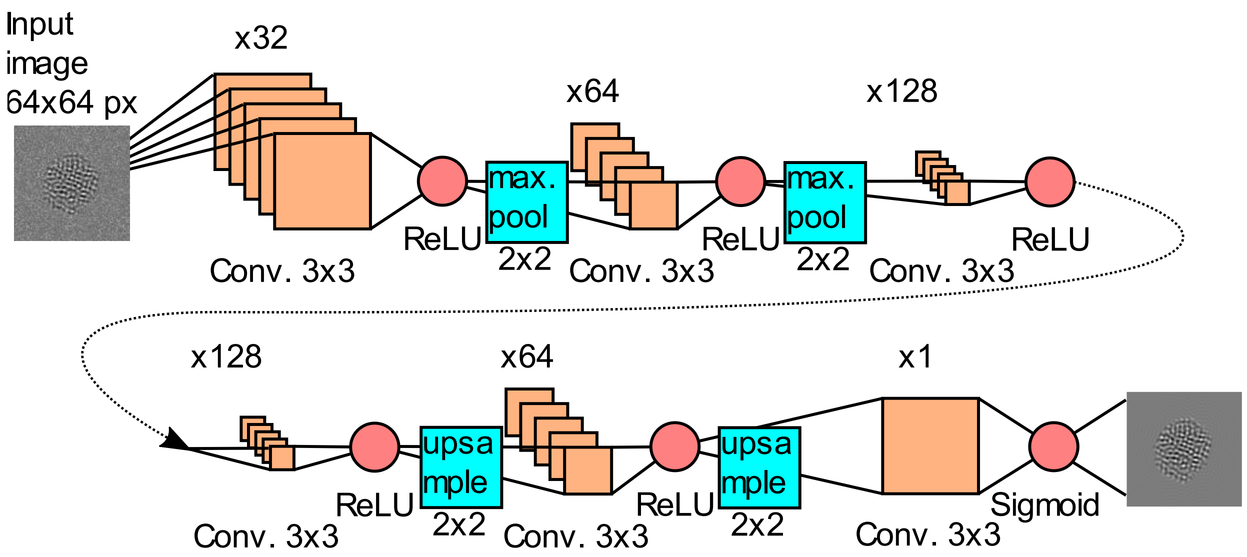
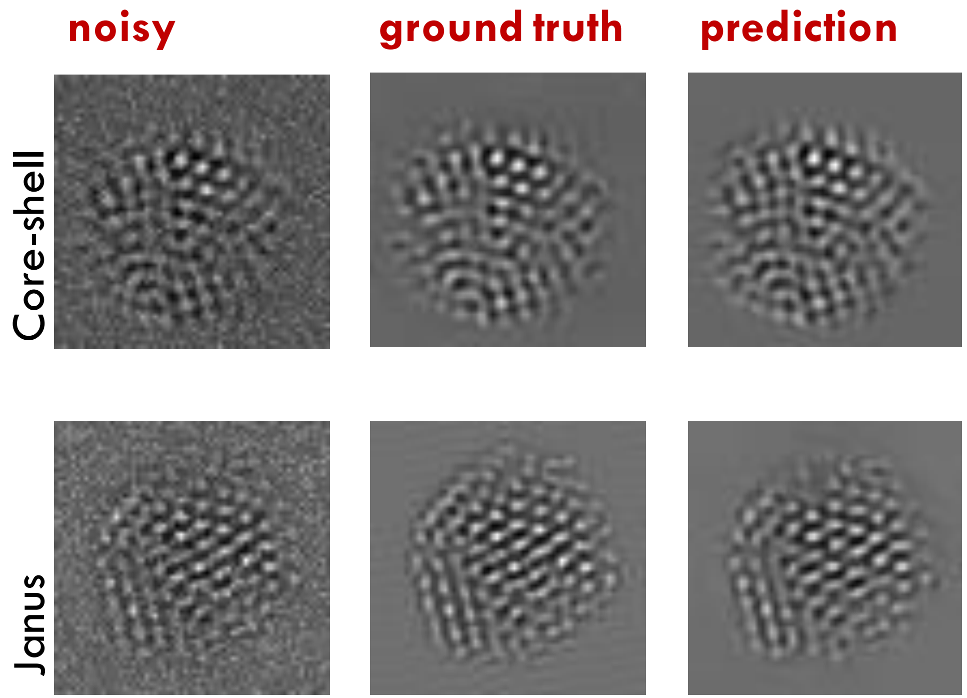


Image denoising

Autoencoder network





➔ almost perfect noise suppression

perspective: **super-resolution**

Conclusion and perspectives

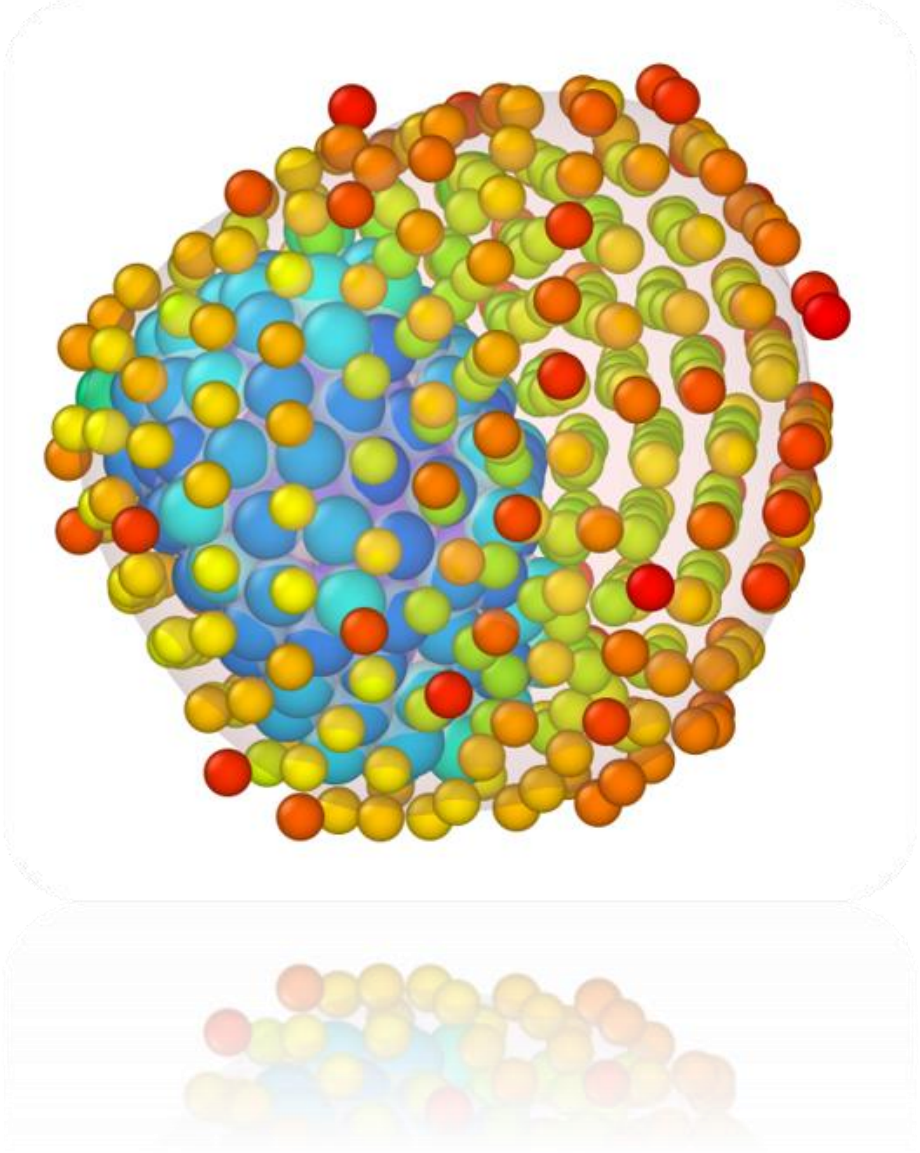
Results

- Classification in terms of chemical ordering: 81%
- Size estimation of particles: ± 33 atoms
- Almost perfect noise suppression

Outlook

- Application to images from experiments

- Other types of analysis, e.g. estimation of microscopy parameters
- Other experimental characterization techniques, such as HAADF STEM, X-ray diffraction, Raman spectroscopy



Many thanks to our collaboration

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Riccardo Ferrando
University of Genoa

Thank you for your attention

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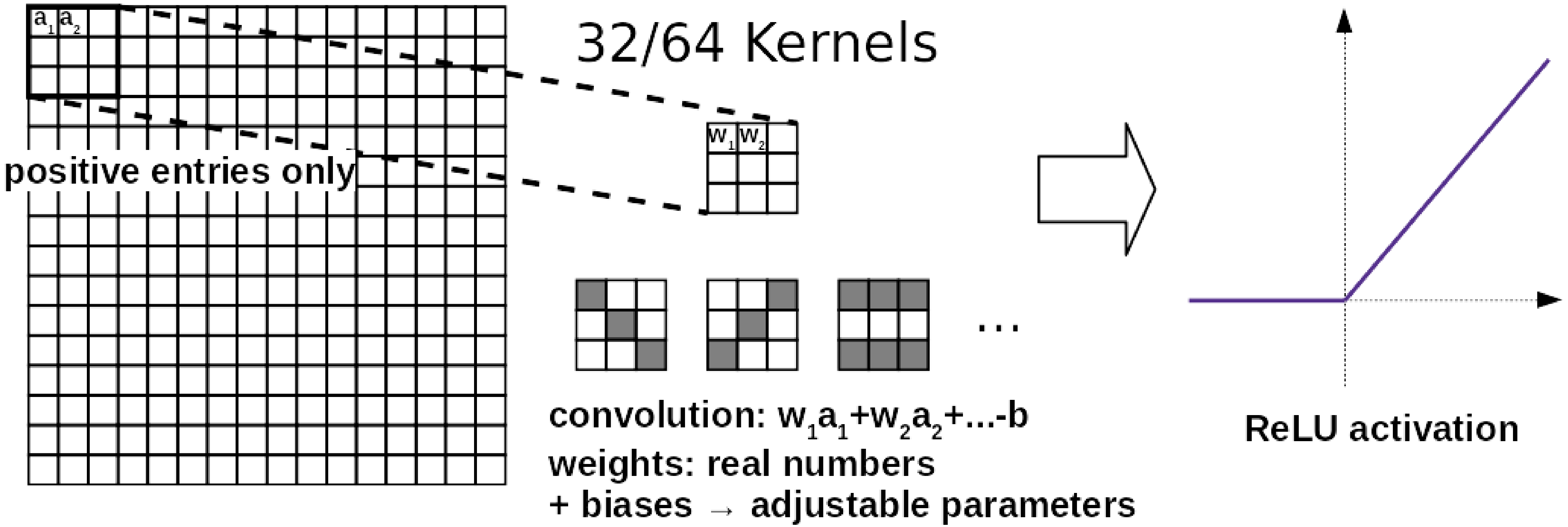
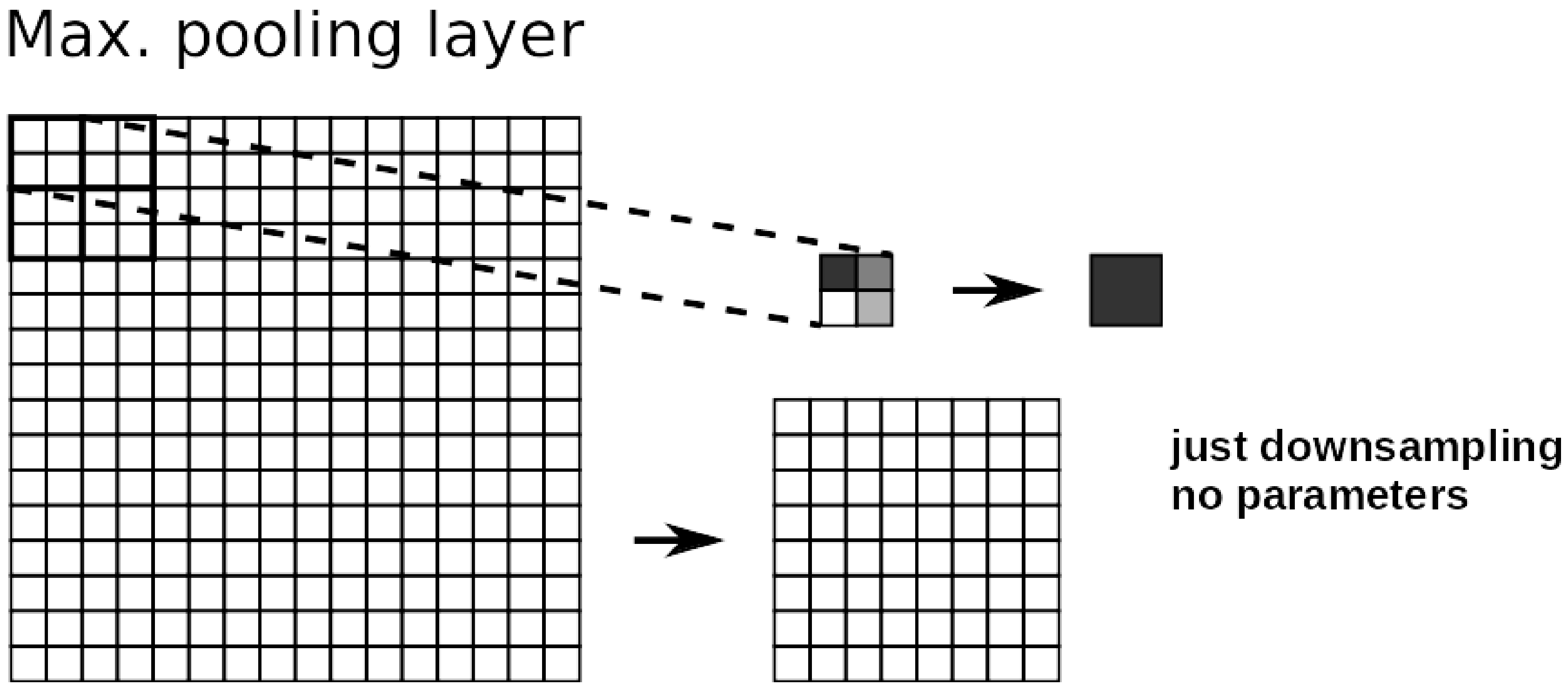
Convolutional neural networks

Convolutional layer



Convolutional neural networks



Convolutional neural networks