



Joseph Davidovits

Nano- Molecular Geopolymer Chemistry

“Advancing new Materials yet to be Discovered.”

Nano-Molecular Geopolymer Chemistry, Advancing new Materials yet to be Discovered.

1) Polymeric character of geopolymers.

The Concept of Geopolymer Micelles.

2) The tiny nanoparticles.

3) Examples of applications.

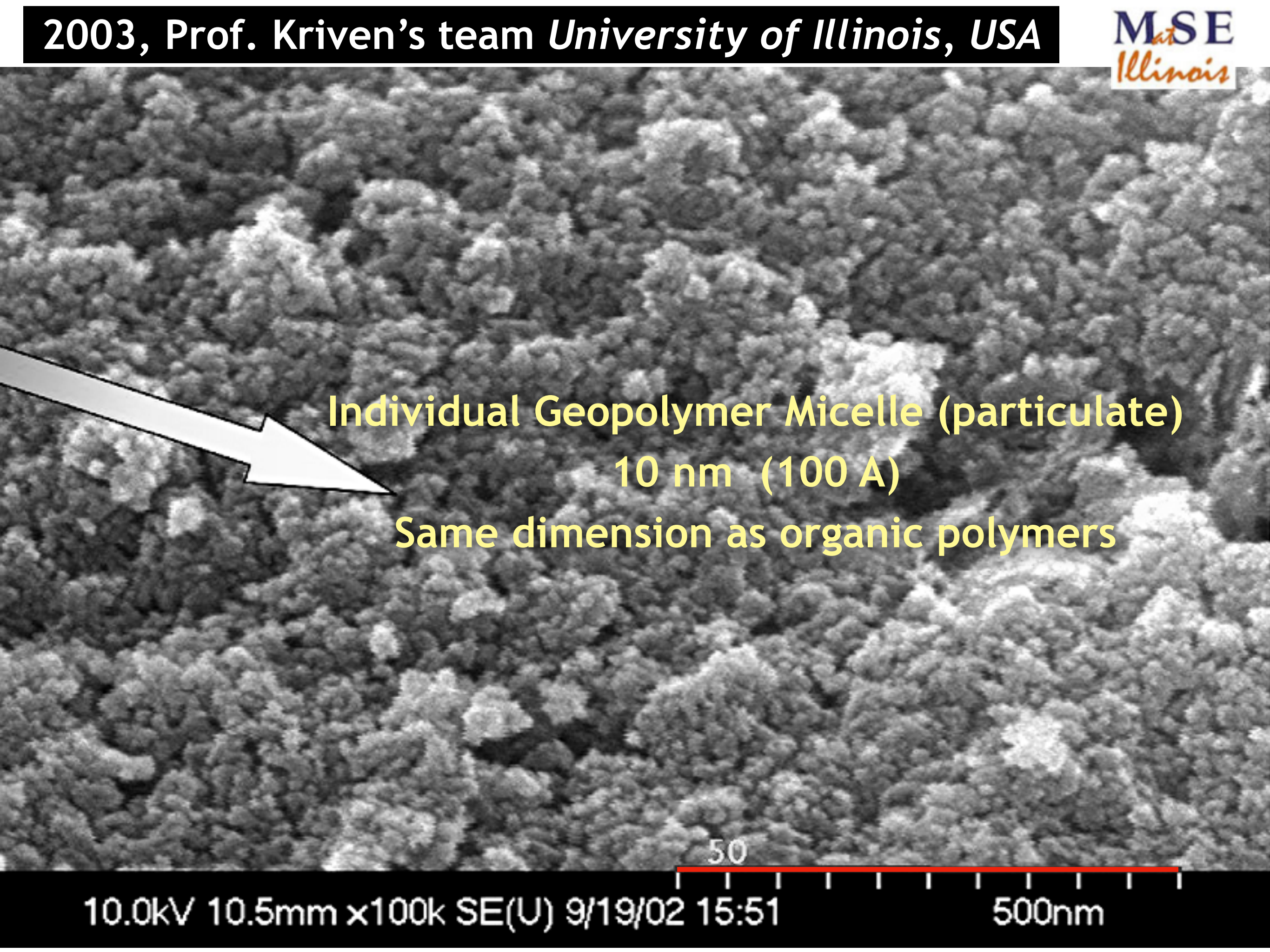
I) Polymeric character of geopolymers.

The Concept of Geopolymer Micelles

“... Joseph Davidovits introduced the term "*geopolymer micelle*" to emphasize the polymeric character of these materials and to describe the fundamental building blocks of the geopolymer structure at the nanoscale.

According to this concept, geopolymerization involves the formation of elementary, discrete nano-sized particles, typically in the range of 10-20 nm.

These nanoparticles are formed inherently during the chemical reaction sequence. The formation mechanism is linked to the polycondensation of reactive oligomers that arise from the initial dissolution of the aluminosilicate precursor...”



Individual Geopolymer Micelle (particulate)
10 nm (100 Å)
Same dimension as organic polymers

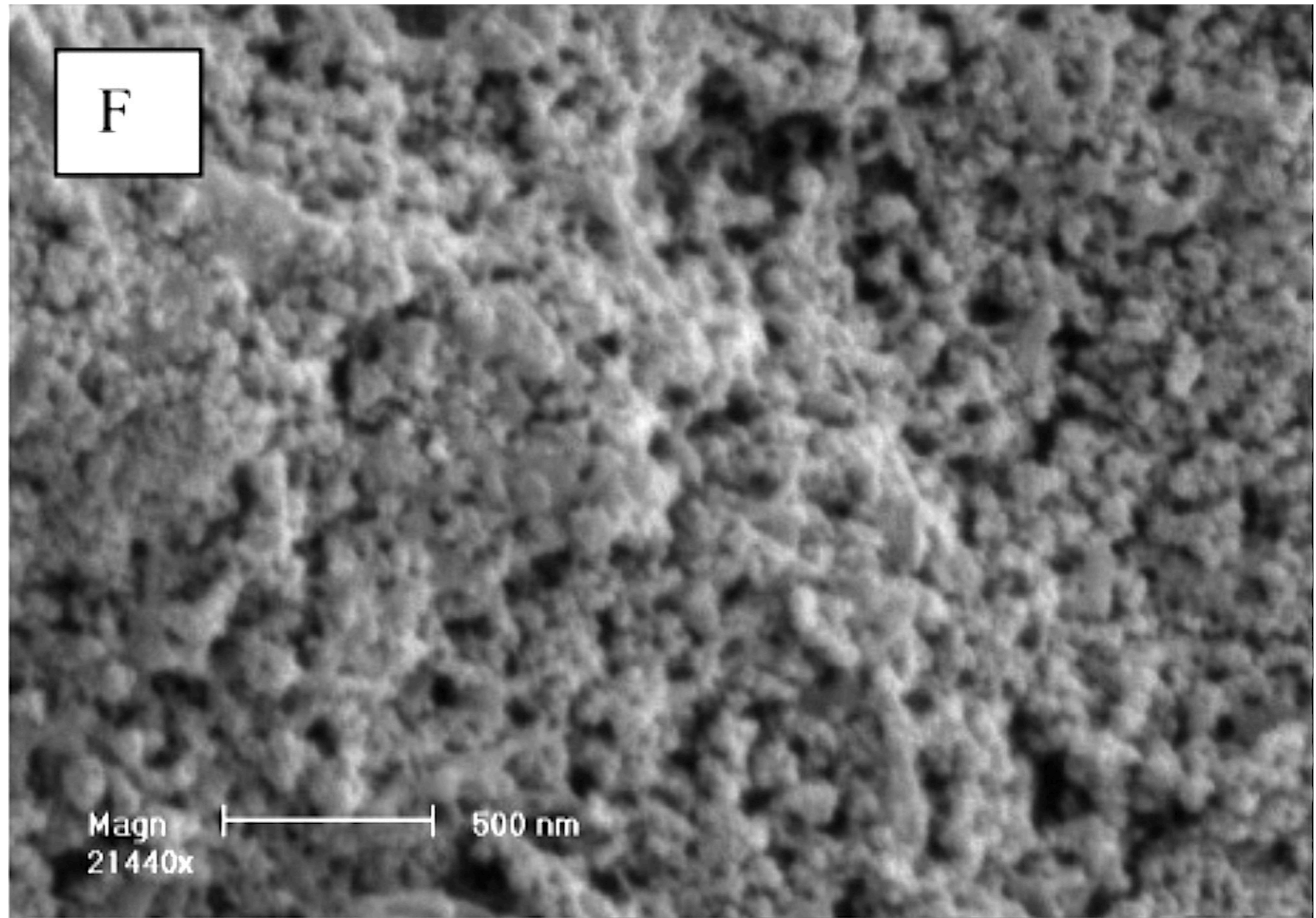
The image is a scanning electron micrograph (SEM) showing a dense field of small, bright, spherical particles. A large white arrow points from the left towards one of these particles. The background is dark and textured.

50

2006: J. van Deventer's team at University of Melbourne, Australia

2006
SEM

Fly-ash based
K-geopolymer
matrix



Effect of Curing Temperature and Silicate Concentration on Fly-Ash-Based Geopolymerization, Sindhunata, J. S. J. van Deventer,* G. C. Lukey, and H. Xu, *Ind. Eng. Chem. Res.* **2006**, 45, 3559-3568.

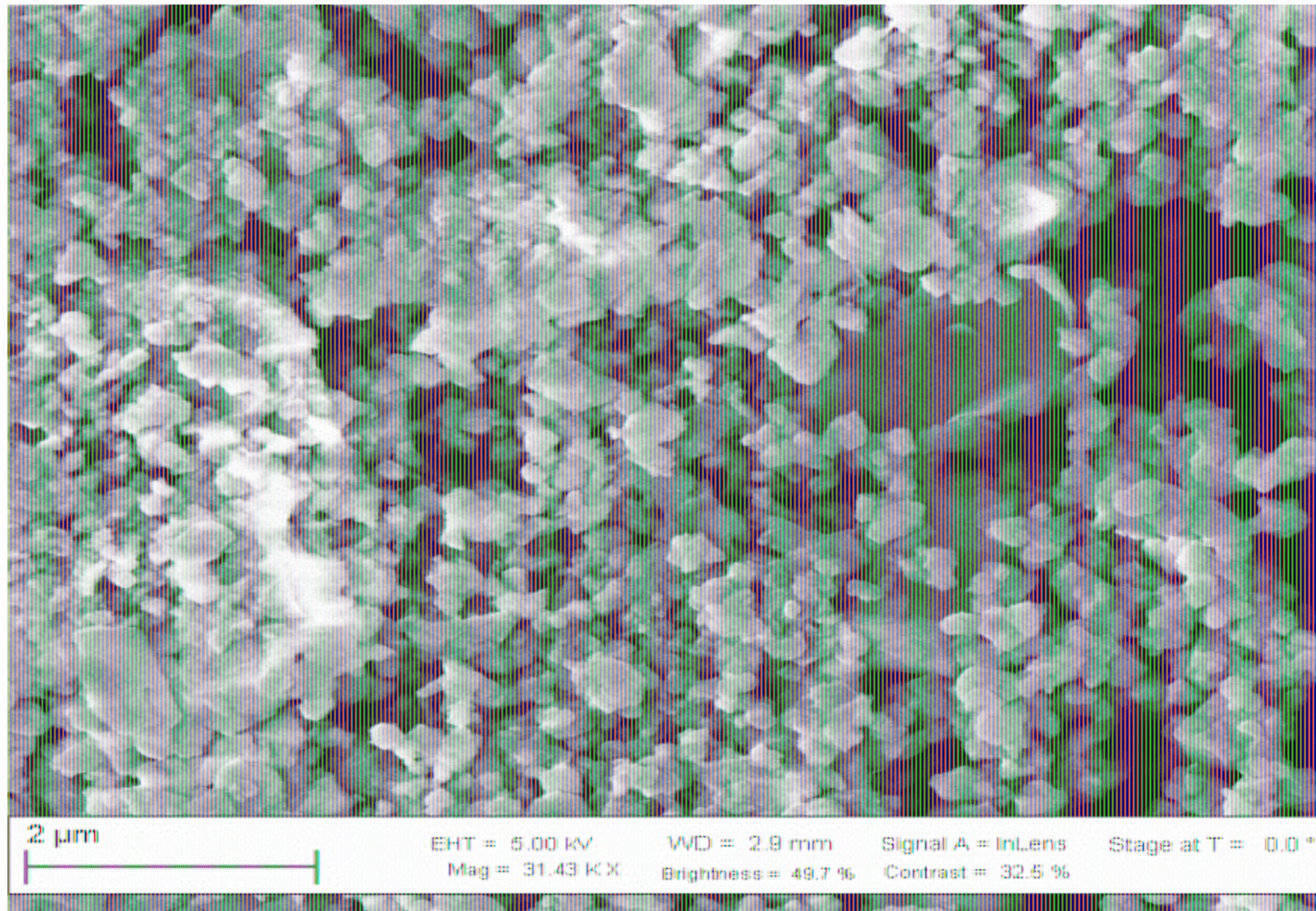
***ECCM15 - 15TH EUROPEAN CONF. ON COMPOSITE MATERIALS,
Venice, Italy, 24-28 June 2012***

*Dražan Jozić, Siniša Zorica, Darko Tibljaš, Sigrid Bernstorff
Univ. of Split, Zagreb, and Sincrotrone Trieste, Italy*

In situ SAXS/WAXS Study of the Developing Process of Geopolymer Structures

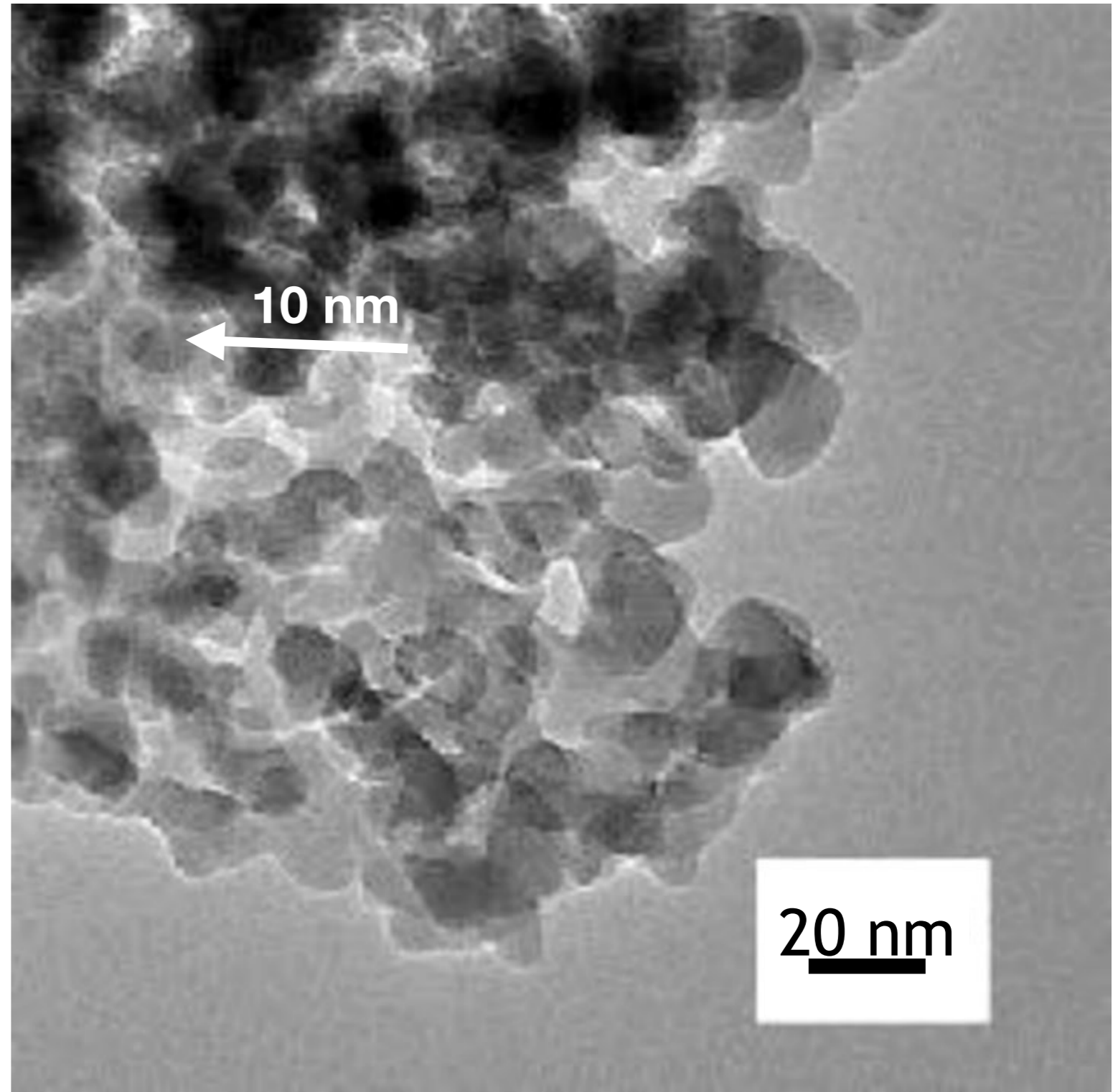
2012
Na-based GP

SEM



2012 Dong-Kyun (Don) Seo's team School of Molecular Sciences,
Arizona State University, Tempe, USA

2012
K-based GP
TEM



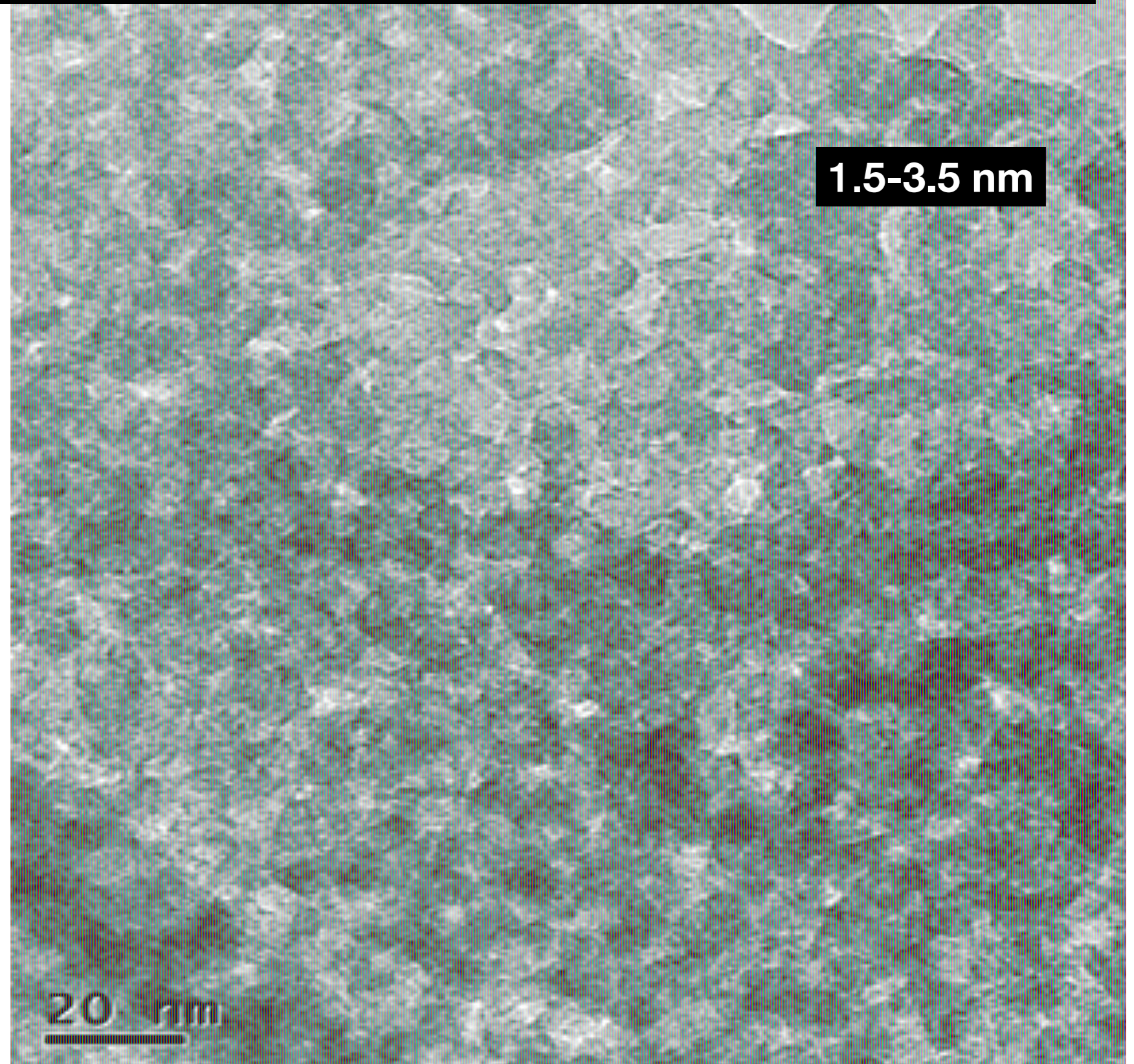
presented at the Geopolymer Camp 2018 under the title: *Nanoaggregates
Synthesis from Low-Temperature Geopolymerization Process*

2) The tiny nanoparticles.

2013: S. Rossignol's team at University of Limoges, France

2013
K-based GP

TEM



A. Autef *et al.*, Influence of metakaolin purities on potassium geopolymer formulation: The existence of several networks, *J. Colloid and Interface Sci.*, **408**, 43-53 (2013)

2023: Geopolymer Institute



meta-kaolinite

Geopolymer-micelles

100 nm



Geopolymer-micelles

10-20 nm

1.5-3.5 nm

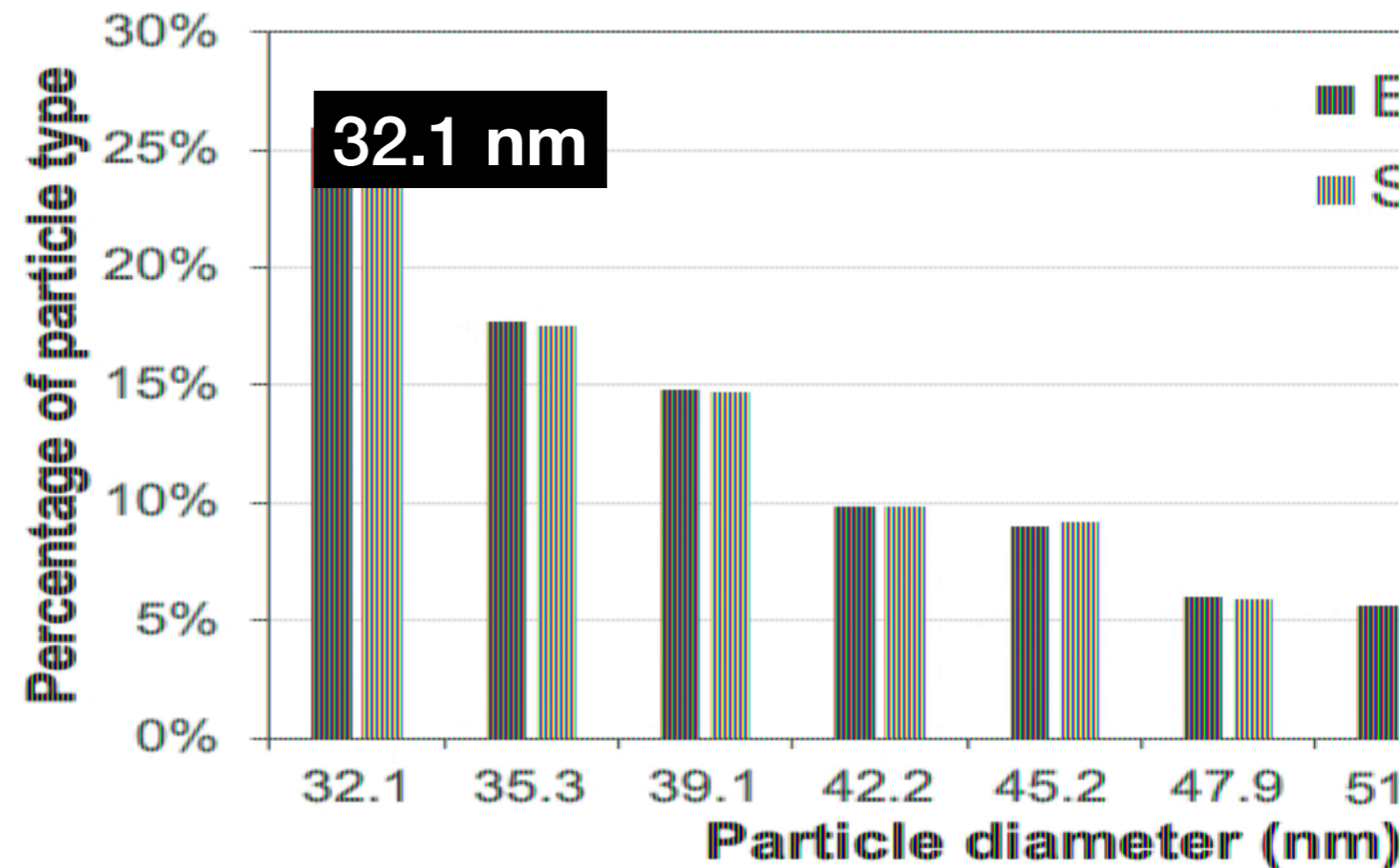
100 nm



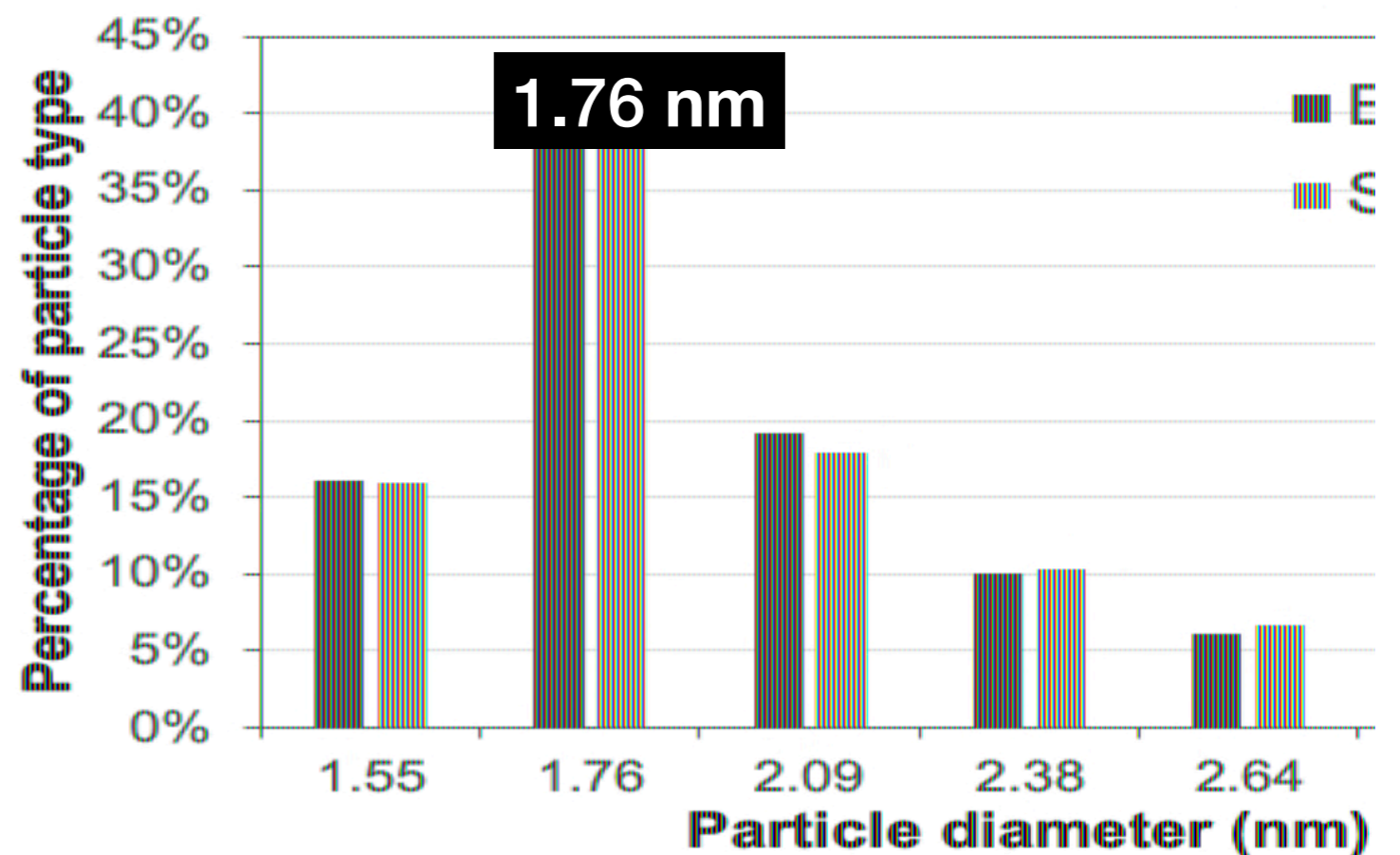
2025: A-T. Prof. Akono's team at North Carolina University USA

Na-based GP-nanoparticles

Adapted from E. Masoero *et al.*,
Nanoparticulates of Sodium
and Potassium Geopolymer
Gels/ Experiments, *Molecular
Dyn* 2025



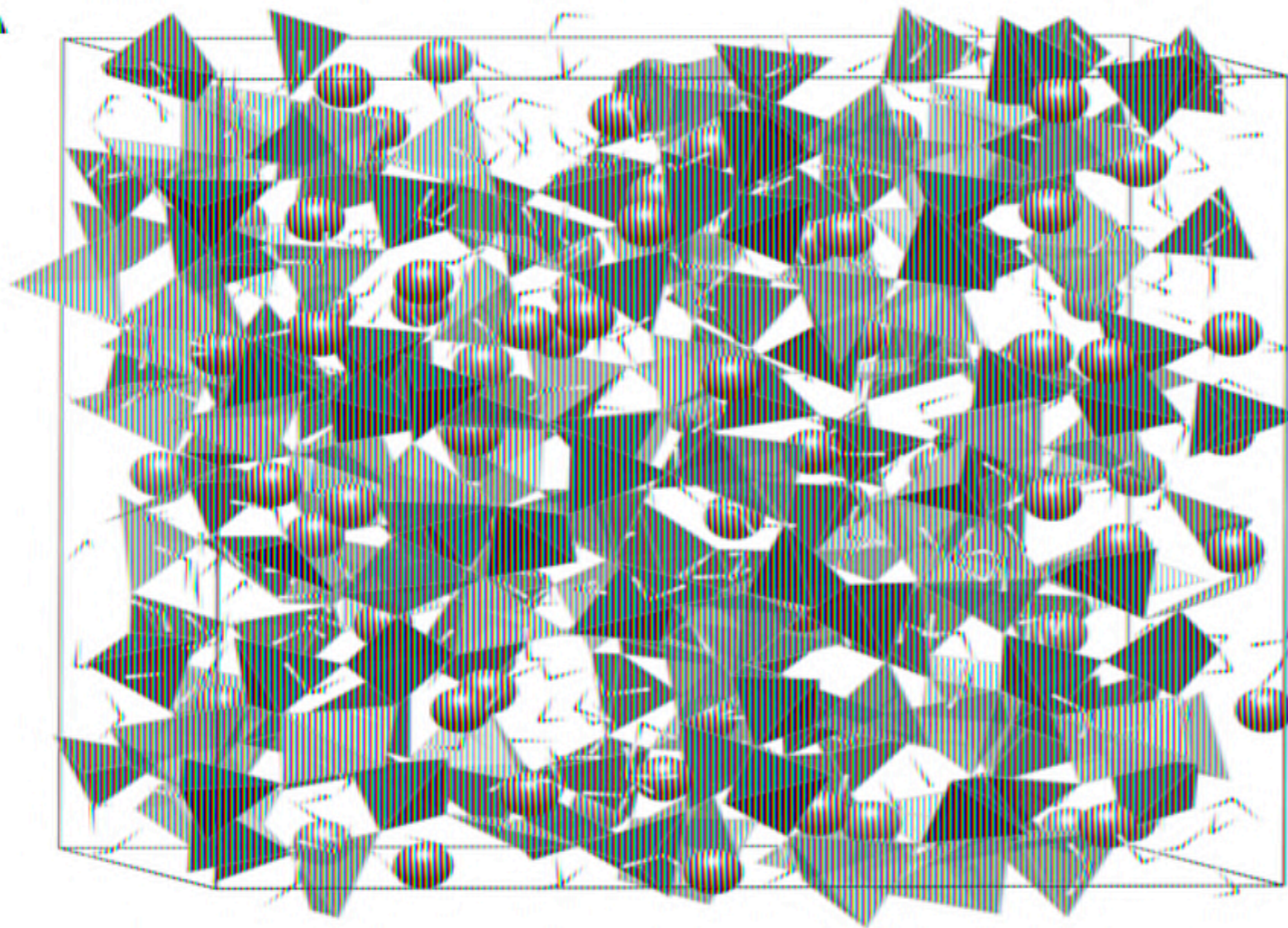
K-based GP-nanoparticles



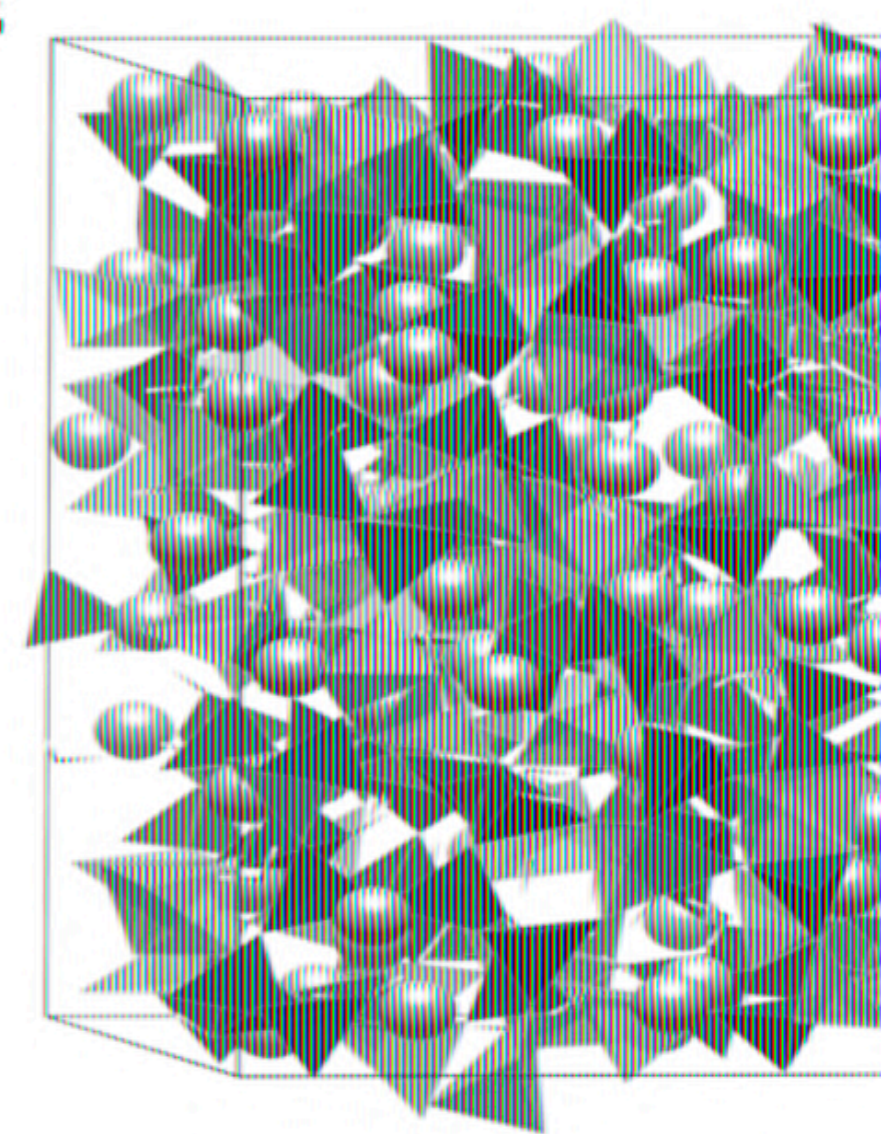
Na-based geopolymer structure

K-based geopolymer structure

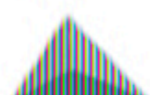
A



B



Silicates



Aluminates



Na ions

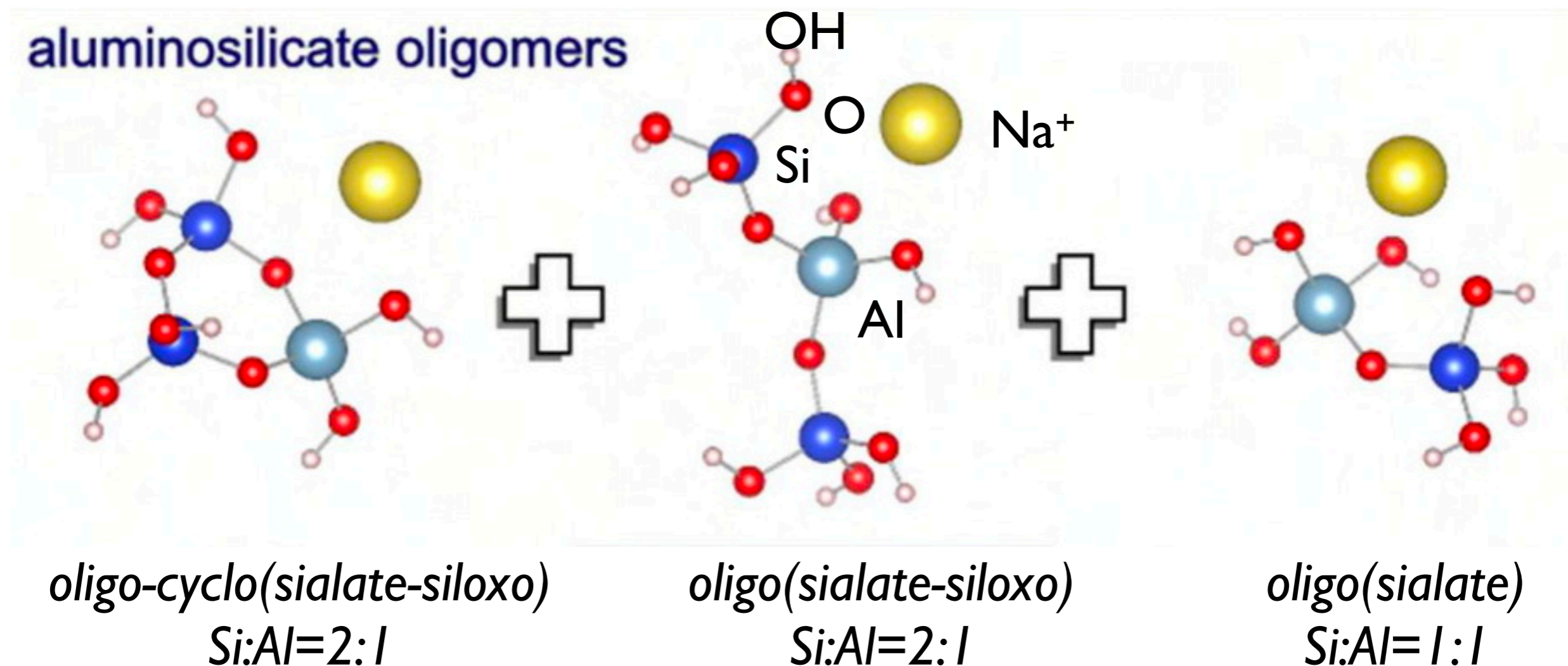


K ions



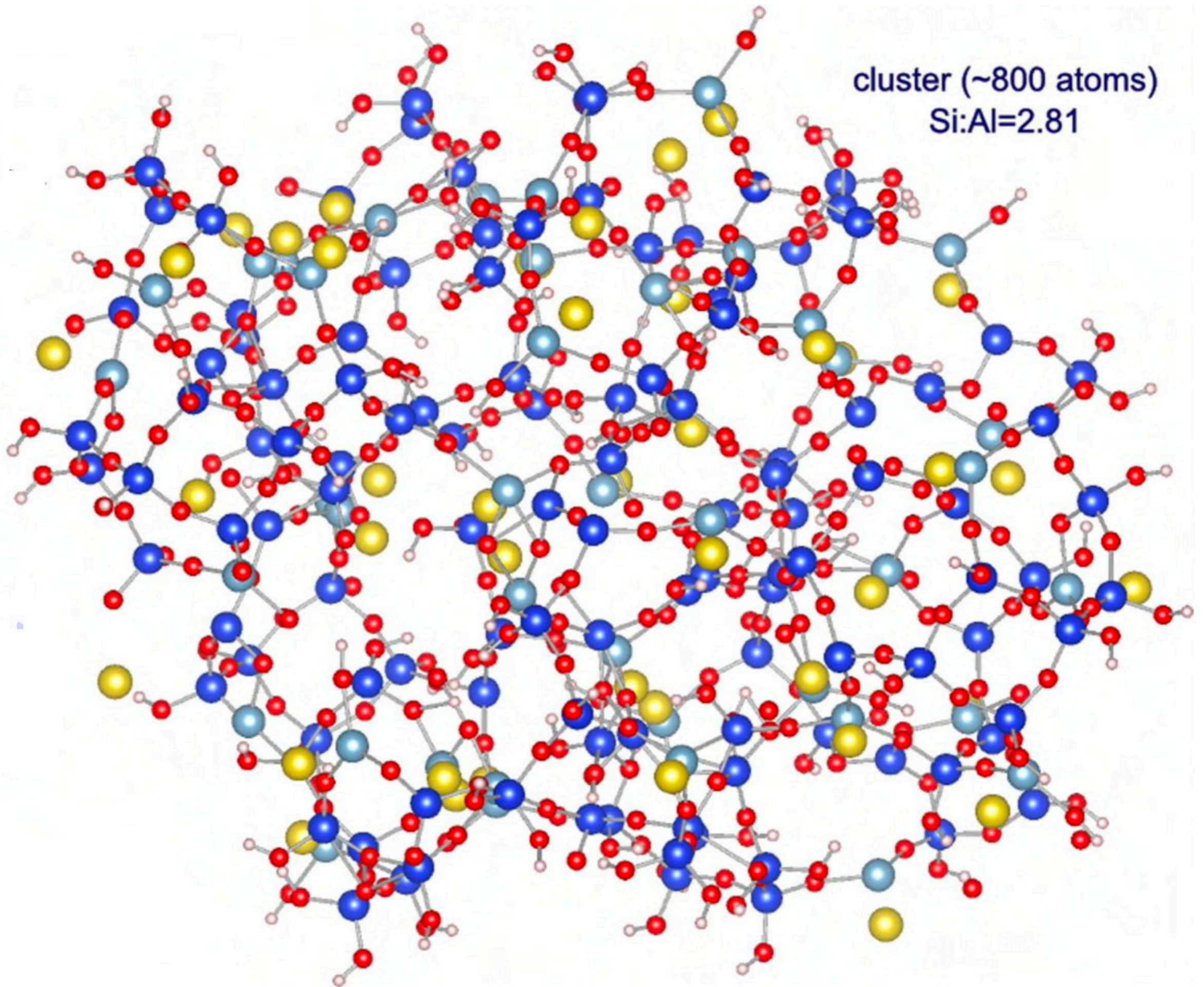
Water molecules

Adapted from E. Masoero *et al.*, Nanoparticulates of Sodium and Potassium Geopolymer Gels/ Experiments, *Molecular Dyn* 2025



A. Koleżyński, M. Król, Mikoł. Żychowicz, The structure of geopolymers – Theoretical studies, *Journal of Molecular Structure* (2018), doi: 10.1016/j.molstruc.2018.03.033.

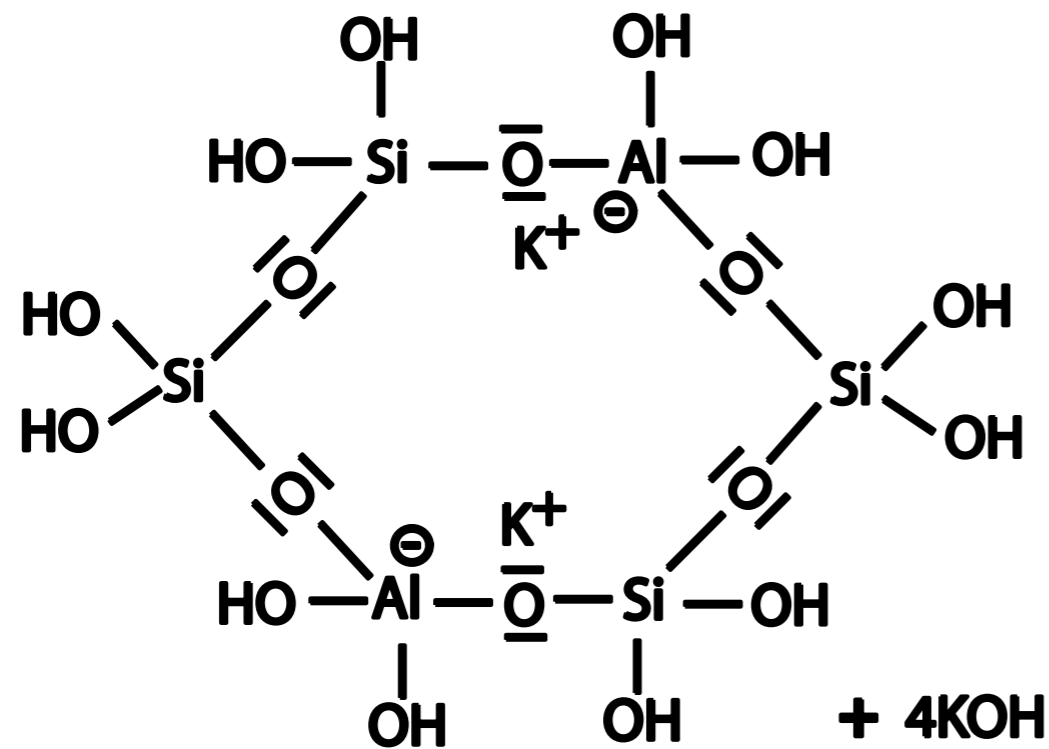
cluster (~800 atoms)
Si:Al=2.81



“....These oligomers act as the monomeric or precursor units that polymerize and cross-link, not into a perfectly continuous gel initially, but into these discrete nanoparticles .The aggregation and further bonding between these primary nanoparticles constitute the “Geopolymer micelles” and the final hardened geopolymer matrix.

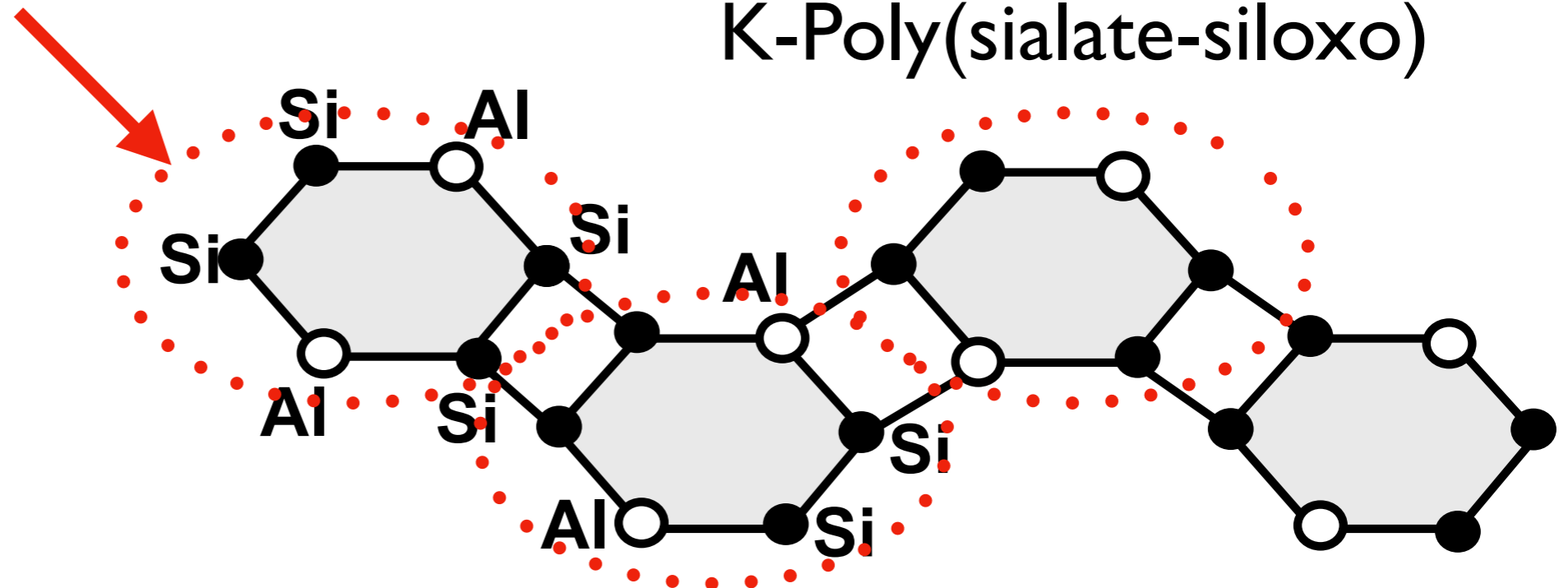
Davidovits distinguishes this model, emphasizing a true polymerization process leading to a well-defined 3D polymeric network built from these nano-units, away from the simpler descriptions that might equate the geopolymer binder solely to an amorphous hydrate gel (like N-A-S-H or K-A-S-H, terms sometimes used analogously by cement scientists)...

Polycondensation of K-poly(sialate-siloxo)



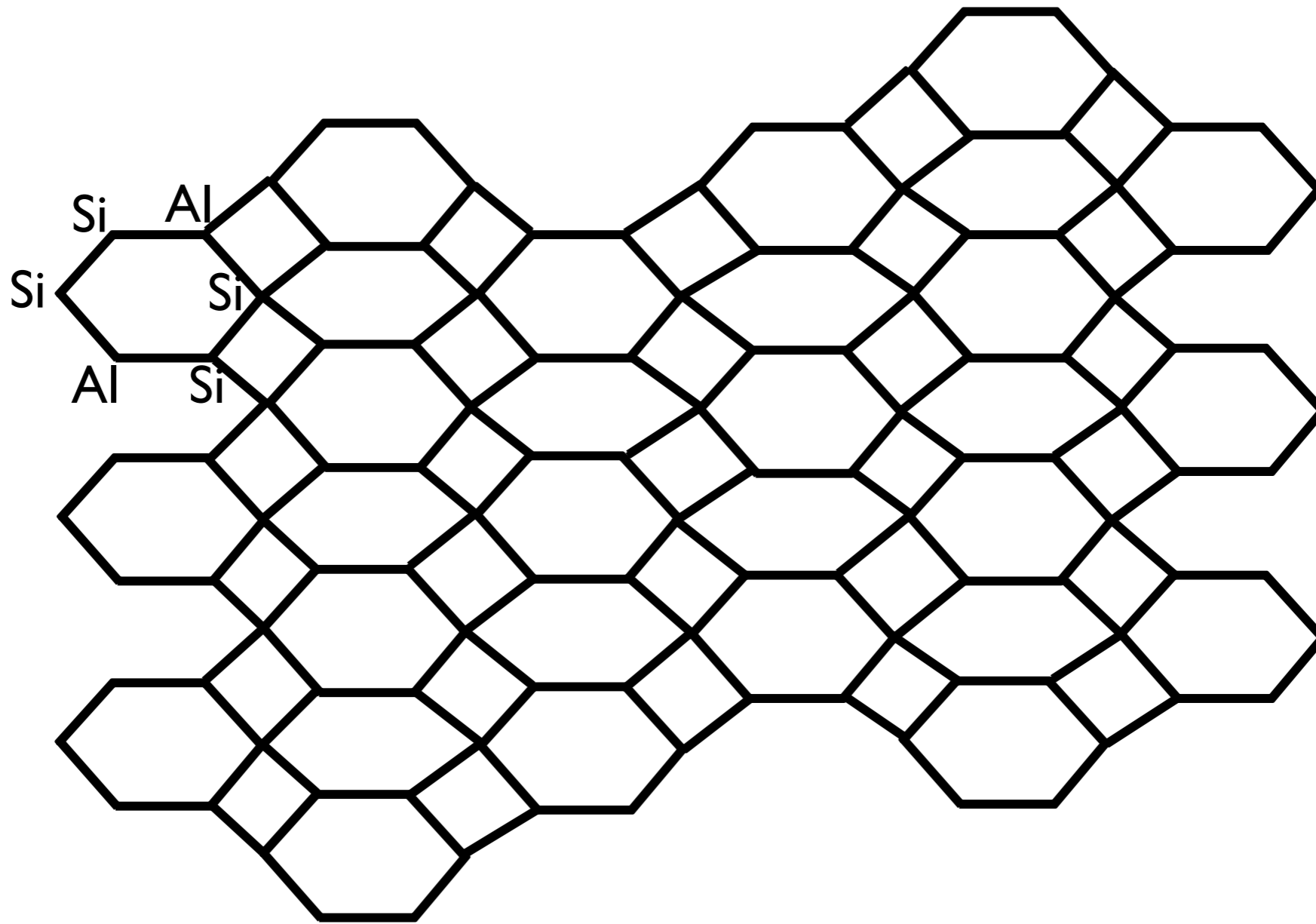
K-oligo(sialate-siloxo)

K-Poly(sialate-siloxo)



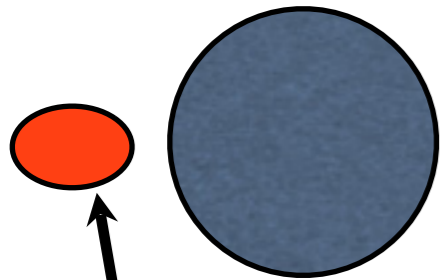
Reticulation, networking of K-poly(sialate-siloxo)

quaternary structure, nano-particles



Leucite framework KSi_2AlO_6

Colloidal
silica
30-40 nm



GP-micelle
10-20 nm

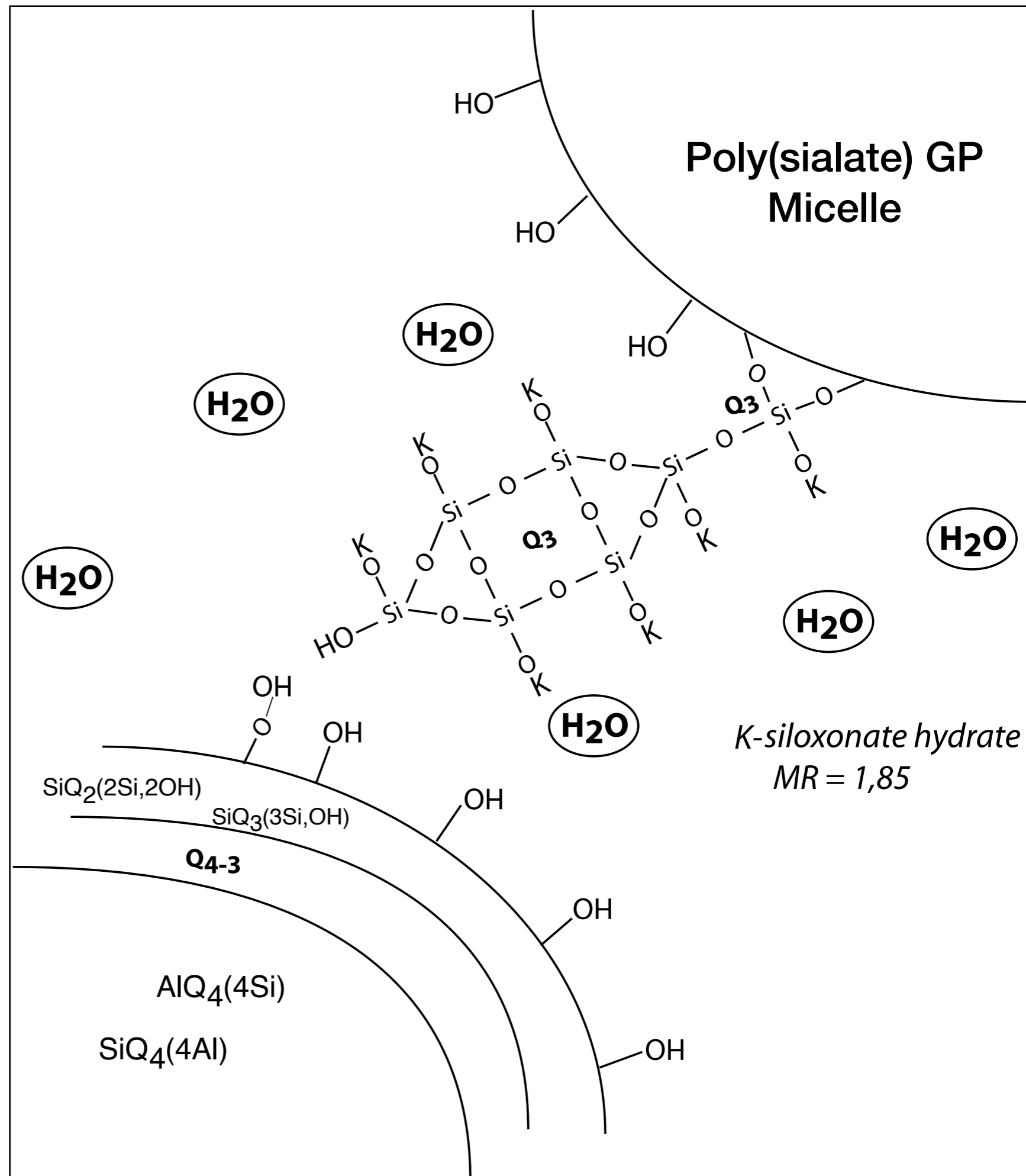
Silica Fume
200-300 nm

Fly ash
3-15 μ

Poly(sialate) Geopolymer = nano material
not unknown « Gel » or « Hydrate »

Inter-micellar
structure after
geopolymerisation.

OH on GP Micelle
surface,
silicate molecules,
water



3) Examples of applications.



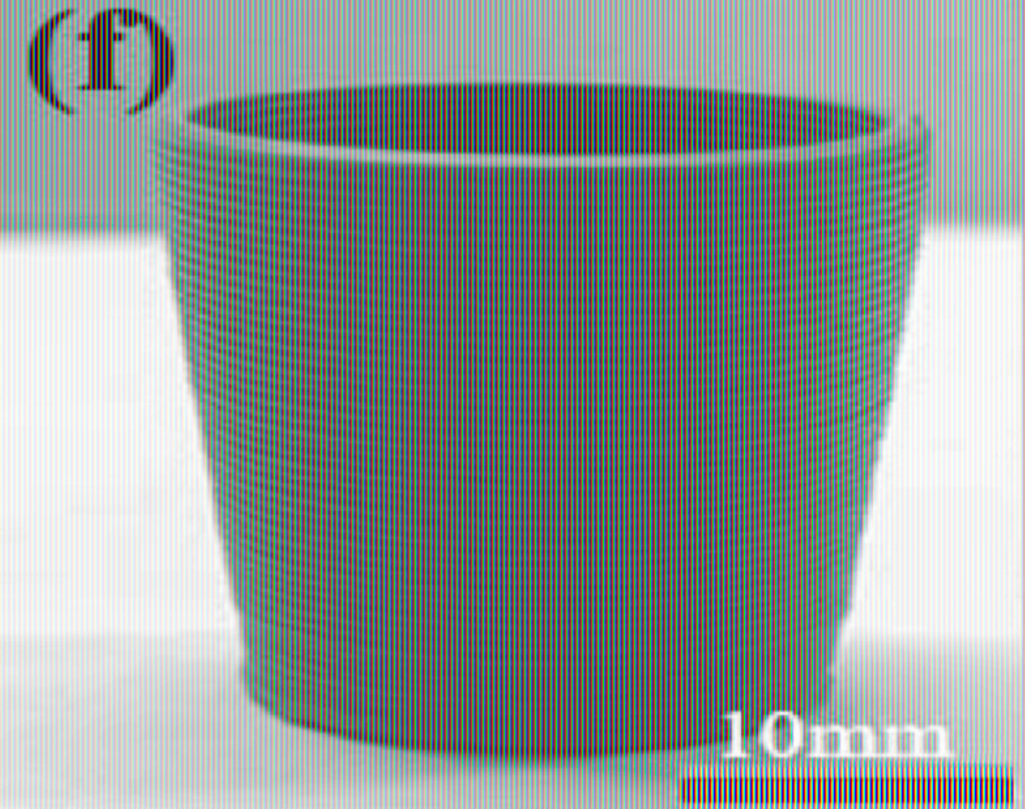
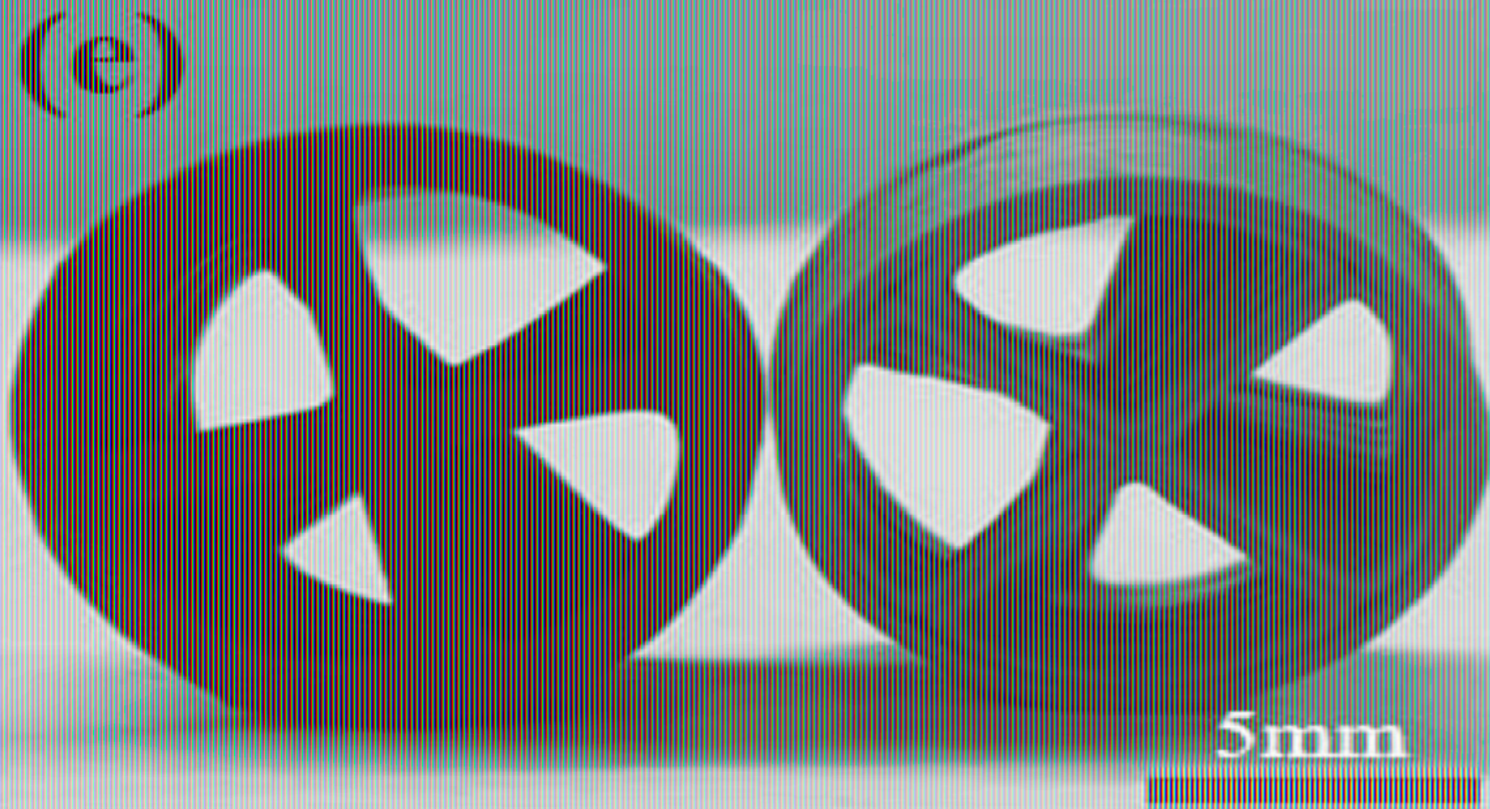
Additive Manufacturing 46 (2021) 102202

Direct ink writing of geopolymer with high spatial resolution and tunable mechanical properties

Siqi Ma, Shuai Fu, Shengjian Zhao, Peigang He, Guoru Ma Meirong Wang, Dechang Jia, Yu Zhou, Harbin Institute of Technology, China.

ABSTRACT:

..... we reveal the mechanism underlying the fracture behaviors of the 3D-printed geopolymers combining compression tests, and theoretical models. Our results pave the way for designing high-quality geopolymer-based materials, which are critical for industrial applications and sustainable development.



(h)

2021 Harbin Institute of Technology, China



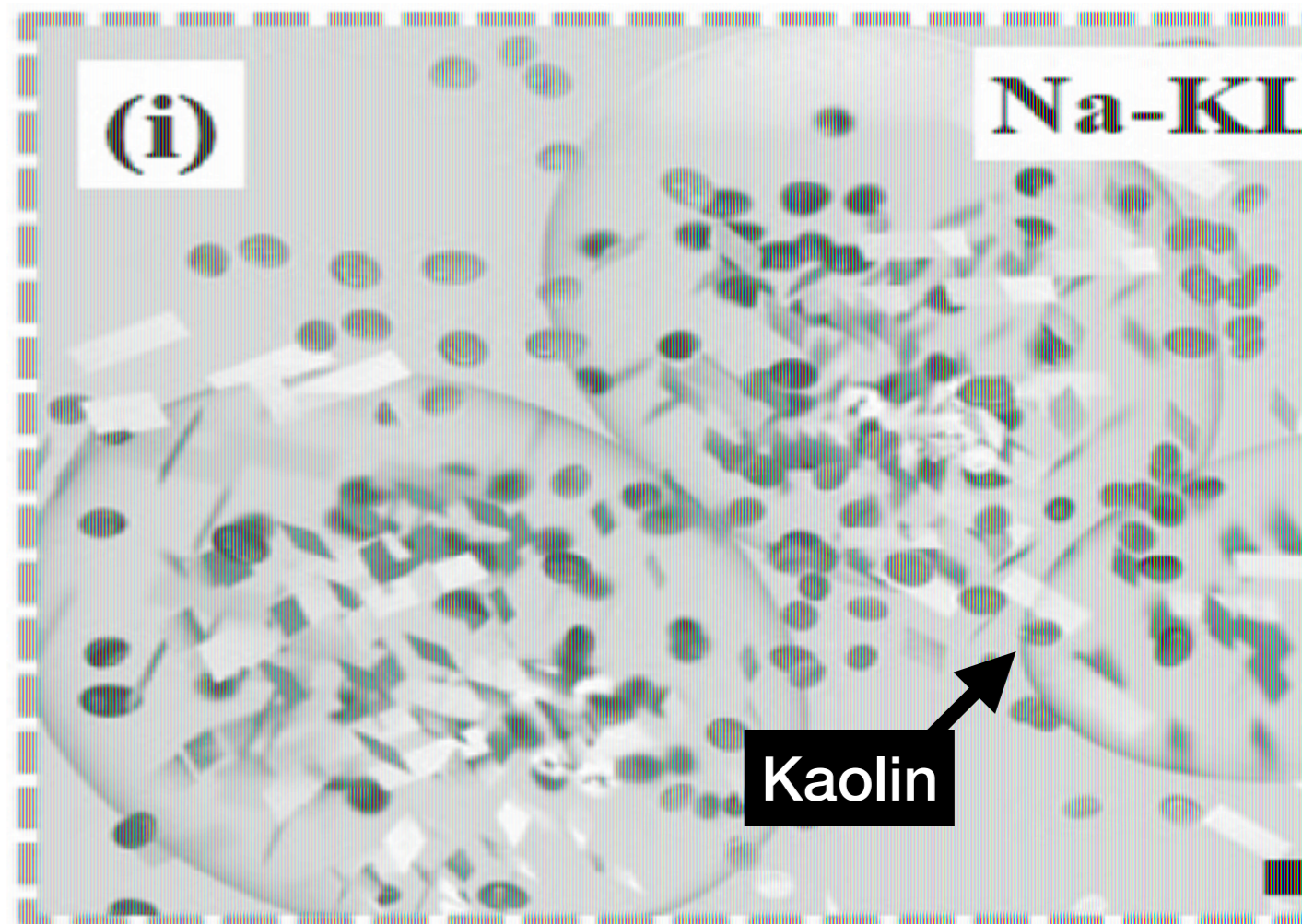
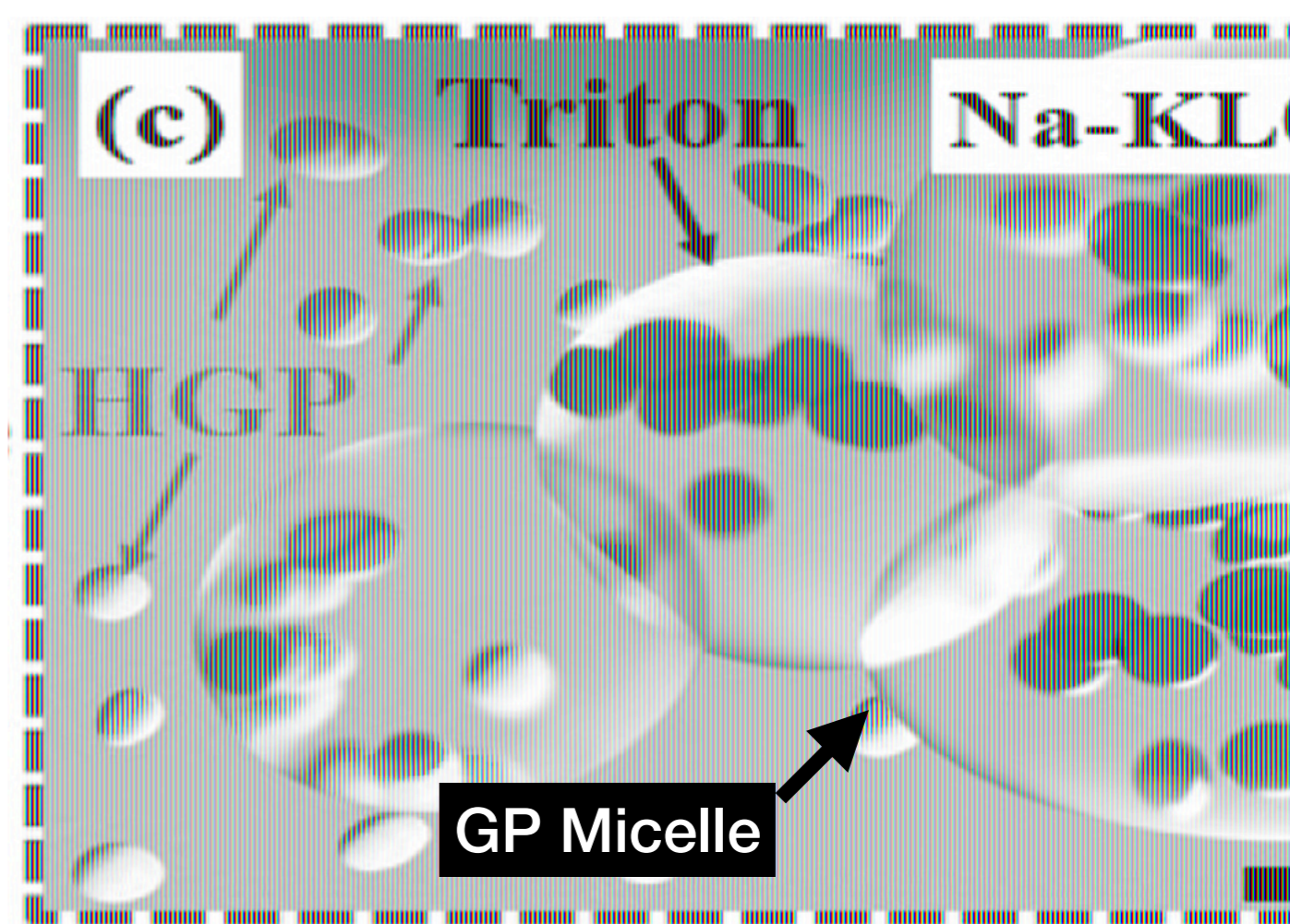
2021

Harbin Institute of Technology China

Encapsulation of Geopolymer Micelles in Triton

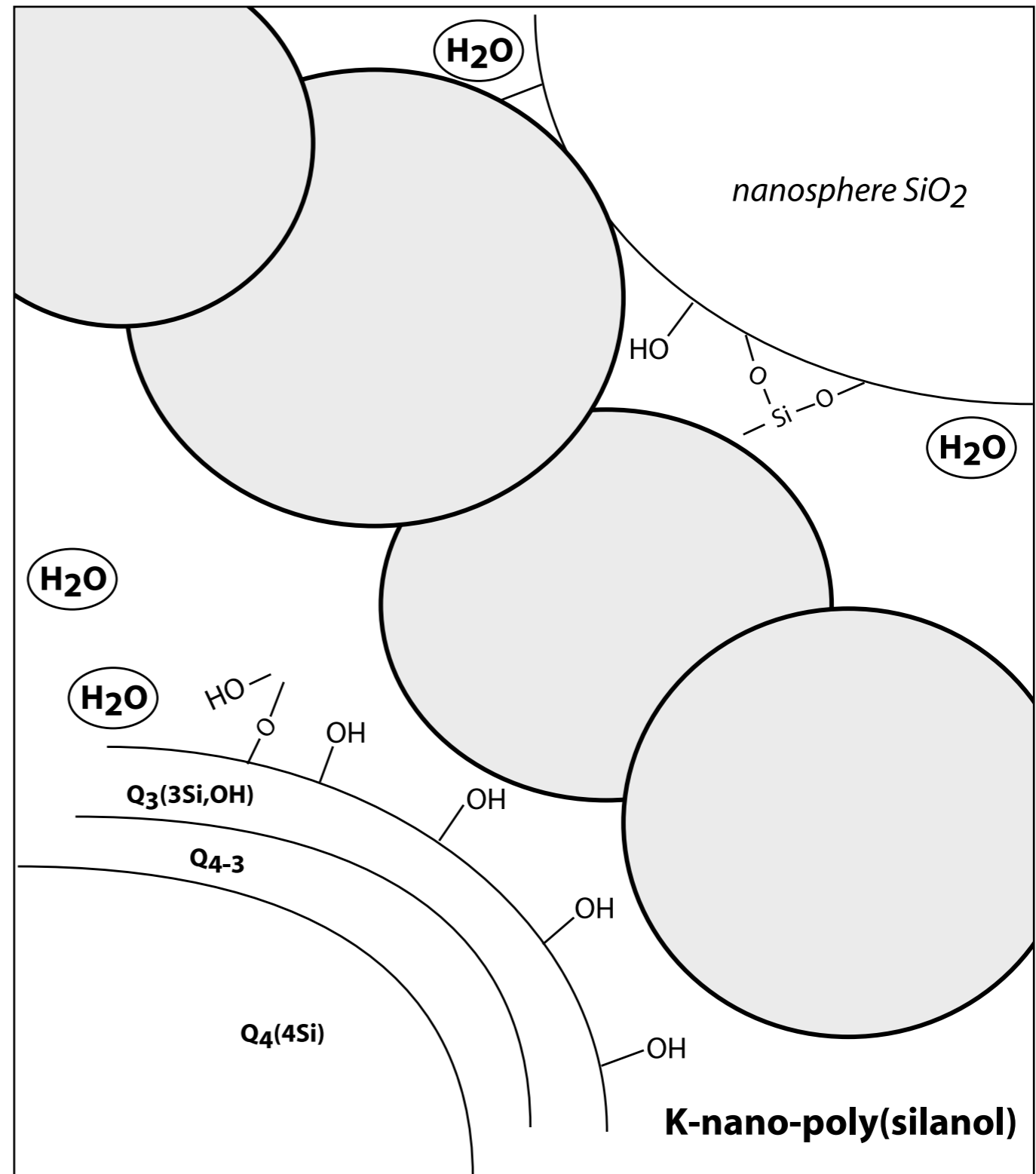
Encapsulation of Kaolin Lamellars with GP Micelles in Triton

(After Siqi Ma *et al.*, Direct ink writing of geopolymer with high spatial resolution and tunable mechanical properties, *Additive Manufacturing* 46 (2021) 102022).



Inter-micellar structure with conductive graphite particulates

Keynote Geopolymer
R&D 2022



The title of this talk was:

Nano-Molecular Geopolymer Chemistry, advancing new materials yet to be discovered.

This was just a brief look at the tremendous potential offered by the structural uniqueness of the Geopolymer Micelle and its Nanoparticle morphology.

I am waiting for new implementations in the very near future.



Joseph Davidovits

Nano- Molecular Geopolymer Chemistry

“Advancing new Materials yet to be Discovered.”