Bionano Interactions Modelling

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Nanoparticles interact with various biological liquids and tissues when coming in contact with the human (animal) bodies.

At different stages of systemic NP distribution one can observe interactions:

1. NP-protein , NP-single lipid interaction
2. NP-NP and NPB-NPB (NPB - biomolecule complex)
3. NP-membrane and NPB-membrane
4. NP-DNA and NPB-DNA
5. NP-glycan
6. Metal ions-cytosol

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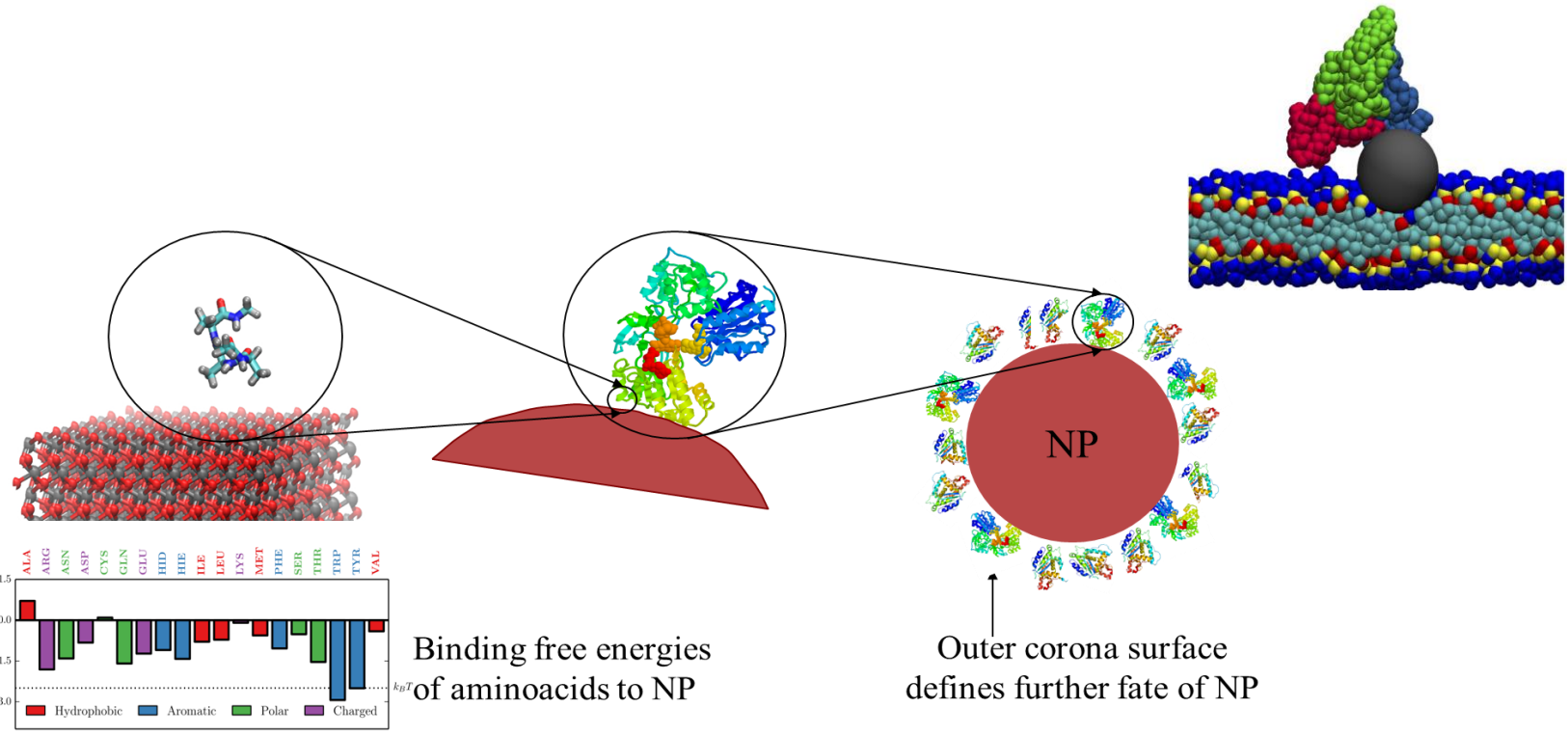
Direct atomistic modelling is unfeasible. Systematic coarse-graining + multiscale simulation needed:

- interaction with biomolecules/membranes, uptake, systemic transport (PBPK), descriptors



Challenges

- Lack of good force fields for atomistic modelling (hard-soft interface)
- Lack of data on hydrophobicity/hydrophilicity of NP surfaces, precision data on the NP coating
- Lack of data on protein/lipid adsorption on NPs, corona content
- Systemic response, long length- and timescales, lysis of corona
- Lack of data on the final state of NP in plasma (single particles, aggregates, etc.)

New approach: focus on initiating events of TPs / AOPs rather than endpoints/cytotoxicity: new descriptors needed.