

- This weeks topics: First we will finish last weeks introduction lecture. We will then start with “Generative Chemistries”: Double Pushout approach, graph grammars, exploring chemical spaces via graph grammars, (sub-)graph Iso-/Monomorphism (Ullmann algorithm), introduction to the first mandatory project.
- Main source of information: Chapter 3 of the PhD thesis by Jakob L. Andersen.
- Mandatory Reading: “An Algorithm for Subgraph Isomorphism” by Ullmann (1976) (see also slide set)
- Recommended Reading: Chapter 1 of “Fundamentals of Algebraic Graph Transformation”: General Introduction. by Ehrig, H., Ehrig, K., Prange, U., Taentzer, G., 2006
- Voluntary Reading: Pages 4-9 of “Algebraic Approaches to Graph Transformation, Part I:” by Corradini et al. (1996)