

- This weeks topics: continue with “Generative Chemistires”: Double Pushout approach, graph grammars, exploring chemical spaces via graph grammars, (sub-)graph Isomorphism (Ullmann algorithm), introduction to the first mandatory project.

- Mandatory Reading: Pages 4-9 of “Algebraic Approaches to Graph Transformation, Part I:” by Corradini et al. (1996)
Mandatory Reading: “An Algorithm for Subgraph Isomorphism” by Ullmann (1976)

- Recommended Reading: Chapter 1 of “Fundamentals of Algebraic Graph Transformation”: General Introduction. by Ehrig, H., Ehrig, K., Prange, U., Taentzer, G., 2006