The actual paradigm shift in the energy sector and the gain in complexity of energy infrastructure and dynamics, particularly in urban environments, demands advanced tools to model, analyze, and optimize these increasingly complex systems. The heterogeneous and interdisciplinary nature of these systems creates the challenge of design holistic approaches to asses them. This dissertation proposes the design and implementation of a modular, interoperable, and scalable ecosystem for the modelling and co-simulation of Urban Energy Systems (UES), with a strong emphasis on automation, standardization, and interdisciplinary collaboration.

The core contribution of this work is the development of the COMES ecosystem, a comprehensive, microservices-based platform. It integrates data acquisition, processing, model generation, and co-simulation workflows for urban-scale energy systems. The ecosystem enables the automated generation of City Information Models (CIM), synthetic networks (e.g., power and district heating), and Functional Mock-up Units (FMUs) from heterogeneous and sparse datasets. Compatibility, modularity, and reusability are ensured by leveraging standard formats and interfaces.

In the ecosystem, simulation is enabled by leveraging co-simulation engines (Mosaik or HELICS). Co-simulation allows the coupling of domain-specific simulators with varying time resolutions and modelling paradigms, enhancing flexibility and interoperability in the framework. It further integrates Reinforcement Learning (RL) compatibility and supports hardware-in-the-loop (HIL) and software-in-the-loop (SIL) experimentation, paving the way for robust, real-world testing of advanced control algorithms and energy flexibility mechanisms.

The proposed ecosystem is validated through five representative case studies:
Urban Digital Twin: Realistic district-scale energy modelling and thermal flexibility assessment in residential buildings.
Power Grid Balancing: Real-time grid management via a hierarchical architecture using multi-agent systems and DR aggregators.
District Heating Systems: Evaluation of thermal storage and flexibility strategies under varying supply temperatures.
Mountain Energy Communities: Co-simulation of rural renewable energy communities including PV, heat pumps, and refurbishment strategies.
DRL for Building Management: Application of deep reinforcement learning for HVAC control optimization in high-performance buildings.

The results prove the ability of the ecosystem to handle cross-domain interactions, support multi-scale and multi-physics simulations, and enable actionable insights for stakeholders. In particular, it is possible to balance fidelity and scalability, addressing both operational and strategic planning needs in urban energy transitions at different scales.

This effort advances the state of the art by providing a reproducible, open, and flexible toolset to facilitate the design, simulation, and validation of smart, sustainable, and resilient city-scale urban energy systems. It is meant to be a core toolset for researchers, policymakers, and industry professionals working in the energy transition.