Explainable-AI-ready materials modelling data and metadata documentation for digital twins and the digital product passport

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This work presents part of the efforts of the Knowledge Graph Alliance (KGA) and its working group for explainable-AI-ready data and metadata principles (XAIR principles WG) in view of metadata standardization efforts and requirements for data-driven modelling and AI systems that comply with the transparency requirements of the AI Act by documenting *epistemic metadata*, *i.e.*, an annotation that helps establish the knowledge status of data [1].
We discuss how the ongoing mid-level ontology development for epistemic metadata [2] can help address such requirements and, beyond this, identify suitable pre-existing semantic artefacts and technologies [3] and the remaining gaps for implementing systems that provide the *digital product passport* as specified (for batteries) by the Batteries Regulation, the Ecodesign for Sustainable Products Regulation, and its future delegated acts. Digital twin infrastructures in manufacturing, *e.g.*, of batteries [4], must be designed to provide the required information.
Based on the KGA's synopsis of core concepts for XAI-readiness [5], we here continue to develop draft actionable core concepts, *i.e.*, definitions of the core concepts jointly with associated concepts, documentation examples, and roles/protocols for such concepts "in action," to help establish both semantic interoperability and pragmatic interoperability [6]. Specifically, the focus of the present work is on establishing "consciousness layer", "neuro-symbolic AI", "scope", "simulation artefact" [5], and "trust" [2] as actionable core concepts.

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