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Integrating Carbon Value Vectors in the Energy and Materials Transition Nexus: A Case Study on Mobility Optimization

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ABSTRACT

The ongoing energy transition involves decarbonization across different sectors. Amongst these, the transportation sector contributes significantly owing to its reliance on traditional fossil fuels as feedstock. Attaining decarbonization goals requires the adoption of novel sustainable technologies such as electric vehicles (EVs), and hydrogen fuel cell vehicles (HFCVs), amongst others. The feedstock transition towards electricity and dense energy carriers is challenged by the requirement for additional infrastructure to manage intermittency, power generation, and grid expansion which requires both materials and capital investment. By evaluating and redirecting the role of carbon value vector from fossil fuel production towards the production of carbon-based materials such as polymers to empower the energy transition, we can optimize resource allocation and maintain economic viability, all while reducing environmental impact. In this work, we propose an integrated framework to systematically address energy-materials-mobility transition nexus challenges. The proposed multiscale framework utilizes a resource-task-network (RTN) representation and a life cycle assessment (LCA) step and considers future material demand and production capacities. Its capabilities are demonstrated through a case study on the transition from gasoline-fueled vehicles to EVs, analyzing (i) the role of carbon value vectors in resources and materials production, and (ii) electricity generation, storage, and dispatch using intermittent renewables. The study reveals the interactions between energy, material, and mobility value chains while providing configurations for exploiting such synergies.

Keywords: Energy transition, Material transition, Carbon value vectors.

INTRODUCTION

The energy transition necessitates the adoption of low-carbon technologies, which are inherently capital-intensive and require substantial material inputs [1]. This creates a critical nexus between energy and materials, as the development of new infrastructure demands significant quantities of resources, while the growing energy sector is required to manufacture components such as wind turbines, solar panels, and electric vehicles [2].

Renewable power systems, such as solar photovoltaics (PV), wind farms (WF), and decarbonized transportation technologies, including EVs, rely on materials like metals, rare earth elements, polymers, and concrete. However, the extraction and processing of these materials are energy and emission intensive [3]. Leveraging synergies between distinct value chains offers a pathway to promote decarbonization while managing economic expenditures.

For instance, polymers have the potential to play a pivotal role in the mobility transition, functioning as carbon sinks, and contributing to decarbonization efforts [4]. We are considering that polymers can be produced from fossil fuels and can be carbon sinks since instead of burning fossil fuels, they can be utilized to produce materials. Another case is when polymeric materials are created from CO_2 captured utilizing CCUS technologies for the current BAU production and utilizing it to produce monomers for polymers through technologies such as methanol to olefins and oxidative coupling of methane. Polymers can enhance fuel efficiency by making vehicles lighter, serve as integral components in renewable energy systems and grid infrastructure, and be synthesized using carbon captured from industrial processes [5]. A promising approach to addressing these challenges involves reevaluating the role of carbon as a value vector. Repurposing existing oil and gas infrastructure for polymer production rather than traditional fuel refinement offers an opportunity to reduce carbon emissions in the mobility sector while capitalizing on existing assets [6, 7].

A holistic approach must be taken to achieve cost-effective solutions in the energy-materials-mobility transition nexus, analyzing the current and future scenarios, and considering all three interconnected aspects to ensure sustainable and efficient outcomes. This includes operational carbon footprint as well as those embedded in material extraction, manufacturing, and infrastructure development. The 3 synergetic transitions in energy, materials, and mobility (See Figure 1), face significant challenges, including managing energy storage for intermittent renewables, addressing emissions from diverse sources, optimizing production costs, and coordinating technology transitions across sectors such as power generation, and transportation [8].

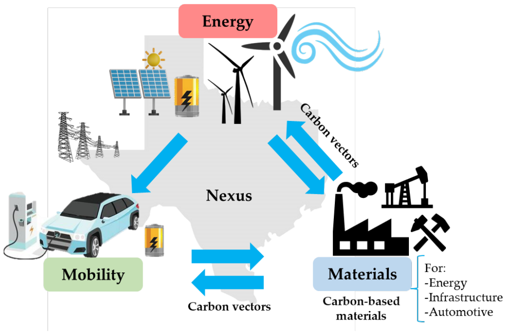

Figure 1. The energy-materials-mobility nexus.

This work introduces a multiscale modeling and optimization framework using the resource task network (RTN) representation which integrates network design and operation considering the nexus between energy-materials-mobility transition. A mixed-integer linear programming (MILP) integrates an LCA step for emissions from material synthesis, resource consumption, and infrastructure establishment. A case study on the transition from gasoline-fueled vehicles to EVs highlights the framework's capabilities, focusing on the role of material production and electricity generation, storage, and dispatch. This analysis implemented in energiapy uncovers synergies between energy, material, and mobility value chains, and identifies optimal configurations, and trade-offs across key parameters [9].

CASE STUDY CONSIDERATIONS

The energy transition is driving a transformation across multiple sectors, including mobility infrastructure, manufacturing technologies, power generation, and material production. These interconnected shifts highlight a crucial nexus between energy, materials, and mobility.

Energy Transition: Power generation must expand to meet the increased demand from transportation and manufacturing. Requisite power generation and management systems can be established through different material alternatives. PVs can be made from monocrystalline or polycrystalline silicon, lithium for lithium-ion batteries can be sourced either through rock or brine lithium, and wind farms can be offshore or land-based each with different material requirements. Other materials required for construction include glass, steel, concrete, aluminum, silicon, copper, and cast iron [10-12].

Material Transition: Low-carbon technologies necessitate the production of advanced materials, such as those needed for renewable energy systems, batteries, and vehicle components. Polymer production is modeled as High-Density Polyethylene (HDPE) production and the production of vehicle parts through a combination of different methods [11].

Technological pathways for plastic production [13]:

1. Business as usual (BAU): HDPE is produced from fossil feedstock such as natural gas and oil.
2. Carbon capture utilization and sequestration (CCUS): Utilizes resources such as CO_2, H_2 and O_2.

Additionally, two processes are given for olefin production from CO_2. The pathways considered for olefin production are [14]:

1. Methanol to Olefins (MTO): Involves synthesizing methanol through CO_2 hydrogenation, which is then converted into olefins, primarily ethylene and propylene.
2. Oxidative Coupling of Methane (OCM): In this process, methane derived from CO_2 hydrogenation undergoes oxidative coupling to predominantly produce ethylene.

Moreover, the role of oil in producing polymers is introduced as a new concept of carbon value vectors utilization of the carbon-based materials that come from fossil fuel production, in which the current oil use for fuels or manufacturing polymers will change over time.

Mobility Transition: This sector involves adopting alternative fuels and transitioning from internal

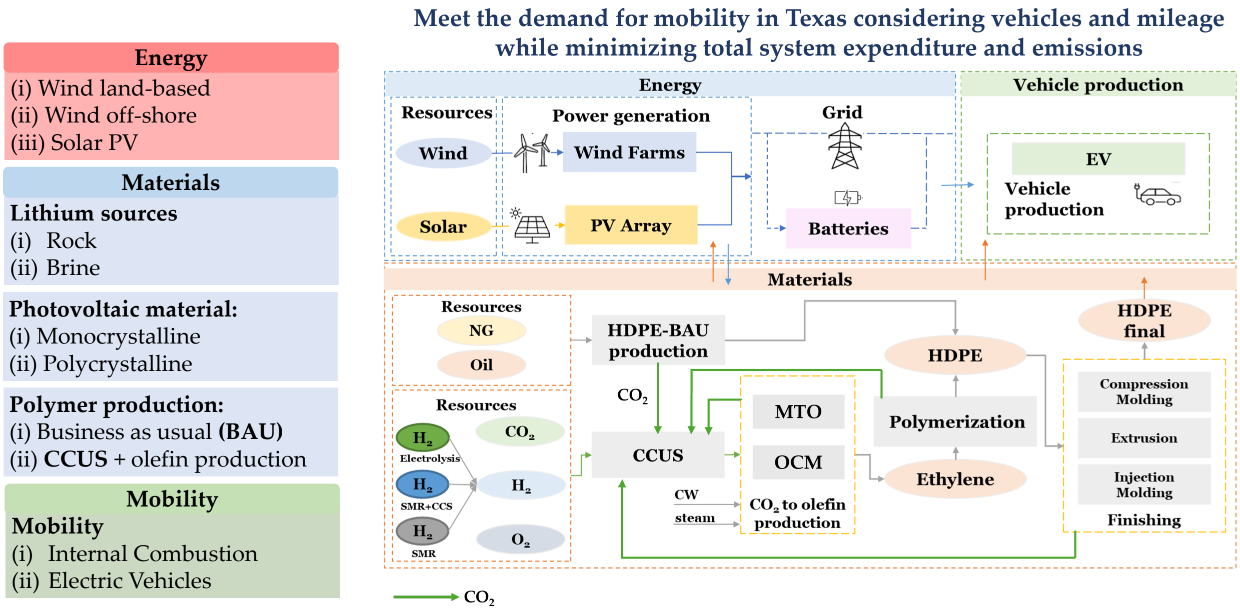

Figure 2: Comprehensive schematic of the mobility transition supply chain case study, illustrating the included resources and processes. The diagram comprises three key components: 1) Renewable energy-based power generation. 2) Polymer production via both fossil fuel-based (BAU) and CCUS pathways. 3) Vehicle production, focusing on three HDPE finishing processes for automotive applications.

combustion engine vehicles (ICEVs) to alternatives such as EVs [15]. This requires both new types of vehicles and the infrastructure to support them.

These transitions are highly interdependent, creating a nexus between them. For example, renewable power generation supports manufacturing and transportation, while advanced materials, including carbon-based polymers, enable the development of efficient vehicles and infrastructure. The mobility sector, in turn, influences energy demand and material production needs, creating a feedback loop within this interconnected system. The representation of the system of study is shown in Figure 2, illustrating the key components of the energy-materials-mobility transition nexus.

METHODOLOGY AND FORMULATION

The framework operates on multiple scales, capturing phenomena that vary across space and time, such as fluctuations in renewable energy availability. Additionally, it integrates operational decisions with network planning into a unified model. The planning horizon is divided into two distinct scales: (1) a broader scale for network-level decisions and (2) a detailed scheduling scale with hourly resolution. The framework integrates the optimization of both network design and process scheduling. Mixed-integer linear programming is employed, binary variables are used for decisions such as process placement and selection of optimal material modes, while continuous variables address mass balance and economic considerations. Key constraints include material balance, emission limits, and network design requirements.

Sets and definitions

Table 1: Sets

sets	definition
$l \in L$	location
$p \in P$	process
$r \in R$	resource
$m \in M$	material
$w \in W$	material modes
$e \in E$	emissions
$t \in T^N$ or $t \in T^S$	network or scheduling scale

Network design constraints

- Process/inventory capacity: Processes and inventories are restricted within specified minimum and maximum capacities ($Cap^{P/S-min/max}_{l,p/r,t}$). The binary variable $x^{P/S}_{l,p/r,t}$ takes a value of 1 if the capacity is expanded during that time and 0 otherwise.

$$Cap^{P/S-min}_{l,p/r,t} \cdot x^{P/S}_{l,p/r,t} \le Cap^{P/S}_{l,p/r,t} \le Cap^{P/S-max}_{l,p/r,t} \cdot x^{P/S}_{l,p/r,t} \forall\, l \in L, r \in R, p \in P, t \in T^N \qquad (1)$$

- Capacity of material mode: The capacity of a process $Cap^{P-W}_{l,p,w,t}$ is determined by the material mode selected for constructing the process. This capacity is constrained by the process's minimum and maximum limits. The binary variable $x_{l,p,w,t}^{P-W}$ takes a value of 1 if the material mode is active, and 0 otherwise.

$$Cap_{l,p,t}^{P-min} \cdot x_{l,p,w,t}^{P-W} \leq Cap_{l,p,w,t}^{P-W} \leq Cap_{l,p,t}^{P-max} \cdot x_{l,p,w,t}^{P-W} \forall\, l \in L, w \in W, p \in P, t \in T^N \quad (2)$$

Binary variables $x_{l,p,w,t}^{P-W}$ are introduced for each process and material mode option used. The binary variable $x_{l,p,t}^{P}$ indicates whether a process is active or not and is defined as the sum of the binary variables corresponding to the selected material modes for that process.

$$x_{l,p,t}^{P} = \sum_{w \in W} x_{l,p,w,t}^{P-W} \,\forall\, l \in L, w \in W, p \in P, t \in T^N \quad (3)$$

Materials constraints

- Materials to set up a process: This quantity ($Mat_{l,p,m,t}^{P}$). is the sum of the products of material consumption ($Mat_{p,w,m}^{cons}$) for a given process, mode, and material, and the capacity of each process mode ($Cap_{l,p,w,t}^{P-W}$).

$$Mat_{l,p,m,t}^{P} = \sum_{w \in W} \left(Mat_{p,w,m}^{cons} \cdot Cap_{l,p,w,t}^{P-W} \right)$$
$$\forall\, l \in L, m \in M, p \in P, t \in T^N \quad (4)$$

- Materials utilized at a location: Calculated as the summation of the materials utilized across all processes.

$$Mat_{l,m,t}^{L} = \sum_{p \in P} Mat_{l,p,m,t}^{P} \,\forall\, l \in L, m \in M, t \in T^N \quad (5)$$

- Materials utilized in the network: Calculated as the sum of the materials utilized across all locations.

$$Mat_{m,t}^{N} = \sum_{l \in L} Mat_{l,m,t}^{L} \,\forall\, m \in M, t \in T^N \quad (6)$$

Emissions constraints

Different types of emissions are identified, such as emissions coming from resources, indirect emissions from materials, and direct emissions from processes [10, 11].

- Emissions from materials: The emissions resulting from materials ($Em_{l,e,m,t}^{m}$) are calculated as the product of the emission factor for that material ($EP_{e,}^{m}$) and the amount of the material utilized at a location and time ($Mat_{l,m,t}^{L}$).

$$Em_{l,e,m,t}^{m} = EP_{e,}^{m} \cdot Mat_{l,m,t}^{L} \,\forall\, l \in L, e \in E, m \in M, t \in T^N \quad (7)$$

Emissions are annualized based on the lifespans of the technologies, materials, and vehicles used in the system. Technologies are designed to last 20 years, while vehicles have a lifespan of 15 years. The total emissions are calculated over the entire lifetime of the system, but for reporting purposes, only the annual emissions corresponding to yearly production are displayed.

- Total emissions at a location: This quantity includes emissions from resources ($Em_{l,e,r,t}^{r}$), materials ($Em_{l,e,m,t}^{m}$), and processes ($Em_{l,e,p,t}^{p}$). The total emissions of the network can be calculated in a similar form to equation 6.

$$Em_{l,e,t}^{L} = \sum_{r \in R} Em_{l,e,r,t}^{r} + \sum_{m \in M} Em_{l,e,m,t}^{m} + \sum_{p \in P} Em_{l,e,p,t}^{p} \,\forall\, l \in L, e \in E, t \in T^N \quad (8)$$

Objective functions

Different objectives can be defined based on the decision maker's motivation, such as the minimization of the cost of the network or the environmental impact.

- Cost: Minimize the cost of the network.

$$Min \sum_{t \in T^N} \propto \cdot\, Capex_t^N + Fopex_t^N + Vopex_t^N \quad (9)$$

- Environmental: Minimize the emissions of the network.

$$Min \sum_{t \in T^N} Em_{e,t}^{N} \quad (10)$$

RESULTS AND DISCUSSION

Polymers for the mobility transition

A base case is established to minimize the system cost for polymer production. The network design for the base case consists of WF, PV, LiI batteries, HDPE production from the BAU pathway, and the finishing processes (Figure 3). With the base case established, the network is optimized for reducing GWP, achieving a maximum emissions reduction of 34.7%. The minimum emissions design favors the WF because it has lower material emissions than PV for energy production and integrates the CCUS with the MTO pathway for polymer production (Figure 4). This reduction corresponds to a 135.63% increase in cost compared to the base case (Figure 5).

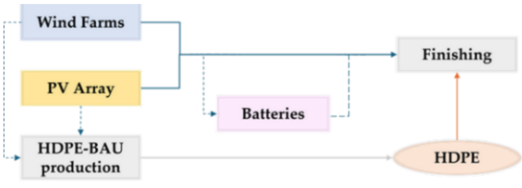

Figure 3. Low-cost pathway for HDPE production.

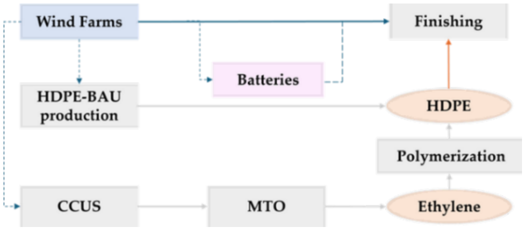

Figure 4. Low carbon pathway for HDPE production.

Integration of materials in the framework

Different studies do not consider the impact of material on the design and scheduling of energy systems, resulting in a more optimistic scenario.

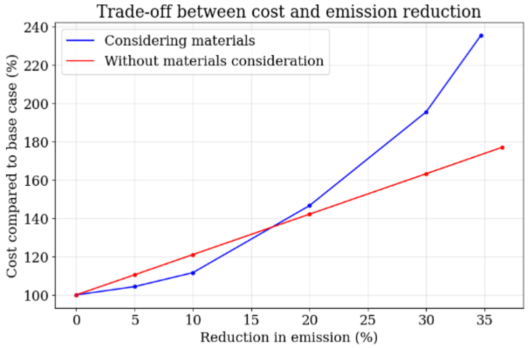

Figure 5. Trade-off between cost and emissions reduction for polymer production.

In this example, including materials results in a maximum emissions reduction of 34.7% with a 135.63% cost increase. However, not including the material aspect in the framework achieved a higher maximum emissions reduction of 36.5% and a lower extra cost (77.1%). These findings highlight the need to account for material aspects to achieve accurate outcomes. Additionally, Figure 6 shows the breakdown of emissions for each point in the Pareto curves above, illustrating the types of materials, resources, and processes that generate emissions in the system.

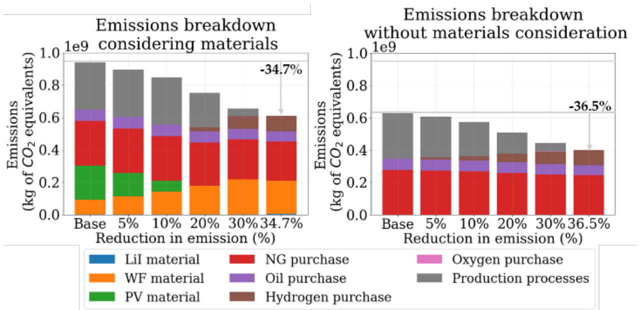

Figure 6. Breakdown of emissions for polymer production.

Analysis of Texas mobility transition through the years

In the last section, only the polymer production for vehicles was considered. Here, the driving phase is also integrated into the case study. For this analysis, the projection of vehicles in Texas was considered with the future demand of cars expected every decade, using a linear model ($y = 305873x - 6 \cdot 10^8$) where y is the number of cars expected in year x. Starting in 2025, with about 26 million vehicles, a base case with all ICE cars is considered. Three scenarios for the future are analyzed, with low, medium, and high reductions in oil consumption.

Table 2: Scenarios studied for mobility transition subject to reduction in oil consumption and EV adoption results.

	Maximum oil consumption (%)					
Scenario	Low (%)	EV (%)	Medium (%)	EV (%)	High (%)	EV (%)
2025	100	0	100	0	100	0
2030	95	12.3	90	18.1	80	29.6
2040	90	27.9	80	37.8	60	55.7
2050 a	85	40	70	52.3	40	74.8
2050 b					0.1	100

For each scenario, the objective is to minimize the cost of the system subject to a maximum hourly consumption of oil concerning the base year 2025 (Table 2). An extra scenario with 100% EVs by 2050 was also introduced (2050 b). The constraints in the reduction of oil consumption led to the adoption of EVs (Table 2), the number of EVs shown corresponds to the minimum cost of the network with energy coming from PVs and WFs.

Cost of the mobility transition

For each scenario, the reduction in oil consumption affected lowering the average emissions per car over the years. Additionally, the average cost per car and yearly emissions were determined as shown in Figure 7. It is shown that the total emissions per car are reduced with a significant cost increase due to the investment in EVs and renewable energy generation. Relying solely on wind farms for power generation incurs higher costs but results in greater emissions reduction due to the lower emissions associated with materials for WFs (Figure 8).

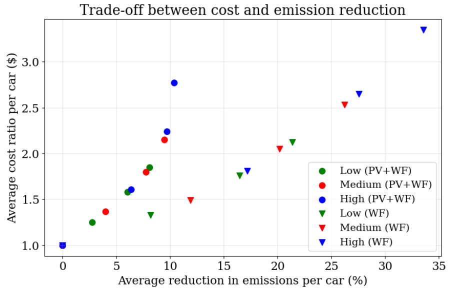

Figure 7. Cost vs. emissions of the mobility transition.

Material impact on the mobility transition

The environmental impact of the mobility transition was quantified by considering materials, resources, and processes, as shown in Figure 8 (for the high reduction in oil consumption scenario). It is important to note that the total emissions of the fleet decrease in cases where all the energy is generated through WF. However, this result depends on the assumption of the fleet projections. For example, despite the adoption of EVs, emissions may continue to rise if energy production relies on a combination of photovoltaic (PV) systems and WFs due to the material emissions associated with PVs. However, emissions will still be lower than solely relying on gasoline vehicles.

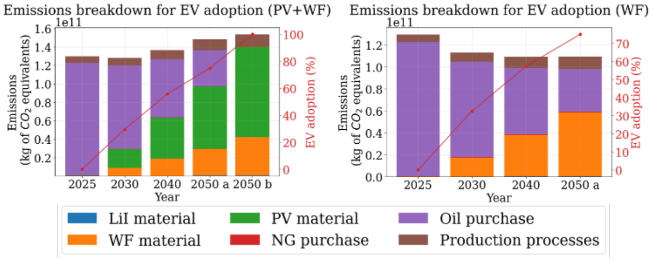

Figure 8. Contribution of materials, resources, and processes to emissions for high EV adoption.

Renewable energy expansion and carbon vectors in the mobility transition

For the given scenarios the total installed capacity of renewable energy was estimated per decade as shown in Figure 9. Additionally, these capacities were compared with the current Texas grid capacity (Table 3), finding that the expansion of renewable energy can be similar to the current installed grid capacity for scenario 2050 b (100% EV).

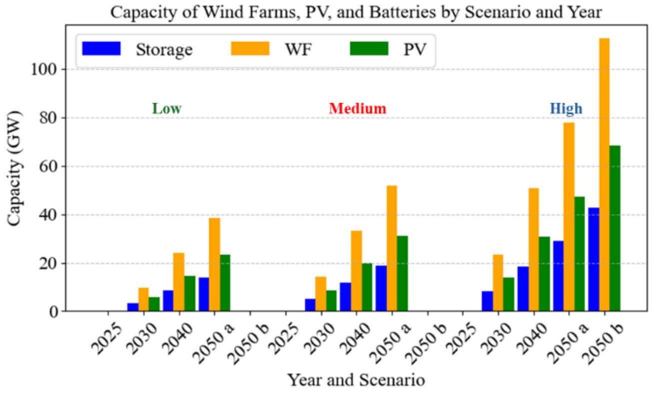

Figure 9. Required installed capacity of renewables and storage for the mobility transition.

Moreover, Table 3 evaluates the carbon value vectors of oil used in producing plastics in the column of oil to plastics, quantifying the amount of oil that can be redirected to valuable polymers for vehicles and charging stations over time. Given that this represents a small amount of the current oil consumption in the mobility sector, other applications for this resource can be explored.

Table 3: Comparison of the required capacity of WF and PV with the current grid capacity in Texas (145 GW).

Scenario	WF capacity (%)	PV capacity (%)	Oil to plastics (%)
2025	0.22	0.14	0.077
2030	16.05	9.67	0.081
2040	34.96	21.11	0.090
2050 a	53.65	32.46	0.098
2050 b	77.56	47.05	0.098

CONCLUSIONS AND FUTURE WORK

This study served to realize interconnections between energy and materials, emphasizing the importance of an integrated energy-materials nexus approach for applications in the design of energy systems. Different aspects were addressed with the framework such as the integration of materials and energy requirements and technologies, the trade-offs between cost and emissions reduction, as well as the impact of emerging technologies. Process lifetimes and the circularity of materials can be incorporated for a more comprehensive approach, as well as carbon taxes and future reductions in EV costs.

Besides renewable intermittency, the framework can also accommodate variability in the cost of resources such as natural gas and oil and resource demand. Case studies considering such aspects and the redirection of oil resources will be presented in future publications. The inclusive framework for the Energy-Materials-Mobility Transition Nexus can coordinate options of technologies and materials to determine the minimum cost, minimum emissions scenarios, and tradeoffs. Considering material use for setting up technology infrastructure systems provides realistic emissions reduction and cost scenarios and allows the investigation of material substitution options as carbon sinks through the utilization of carbon value vectors in a circular economy framework.

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