SUMMARY

[0004] Techniques are provided (e.g., a method, a system, non-transitory computer-readable medium storing code or instructions executable by one or more processors) for managing reuse of molecular components incorporated in waste materials.

[0005] In particular, techniques may be directed to characterizing chemical or material identities of constituent materials entering a waste stream. The constituent materials may be identified using chemical fingerprints derived from a comprehensive library including spectrum information, physical properties, computational algorithms, and machine learning. Material characterization data may be used to develop chemical processes that transform the materials into target products. Identification of the target products and processes can be informed by logistical information, market data, and real time exchange data. For example, target products may be identified as ones associated with relatively high market demand and that can be relatively efficiently produced using at least one the constituent materials.

[0006] According to a first aspect of the present disclosure, there is provided a method including: accessing characterization data of a feedstock, the characterization data including one or more spectra collected according to one or more spectroscopic methods; predicting, using the characterization data, a set of constituent materials included in the feedstock; predicting a material composition of the feedstock using the predicted set of constituent materials; identifying, at least in part using the predicted material composition of the feedstock, one or more target products; generating a set of chemical reaction schemas enabling a conversion of at least part of the feedstock into the one or more target products; storing identifications of the material composition of the feedstock, the one or more target products, and the set of chemical reaction schemas in a data store; and directing a portion of the feedstock to a materials recycling facility configured to convert the portion of the feedstock to at least one target product of the one or more target products.

[0007] In some embodiments, the method may also include identifying one or more inputs to a fitness function, the one or more inputs describing a chemical reaction scheme of the set of chemical reaction schemas. The method may also include generating an output of the fitness function using the one or more inputs. The method may also include selecting an implementation scheme from the set of chemical reaction schemas according to the fitness function, the one or more inputs, and the one or more target products. Identifying the one or more target products may include accessing inventory information describing a set of products and identifying an incomplete subset of the set of products as the one or more target products using the inventory information. The inventory information may include one or more of a quantity of the feedstock

available for conversion or a quantity of a target product of the one or more target products available in a geographical region. Generating a set of chemical reaction schemas may include accessing a chemical reaction inventory, the chemical reaction inventory including representations of chemical reactions describing a conversion of the feedstock to a target product of the one or more target products and populating the set of chemical reaction schemas from the chemical reaction inventory. Generating the set of chemical reaction schemas may include simulating a first constituent reaction of a chemical reaction scheme of the set of chemical reaction schemas using a machine learning model. Generating the set of chemical reaction schemas may include estimating an output of a reward function, with an output of the machine learning model serving as an input to the reward function. Generating the set of chemical reaction schemas may also include estimating a maximum of the reward function by modifying an input to the machine learning model, wherein the input is an output from a second constituent reaction preceding the first constituent reaction in the chemical reaction scheme.

[0008] According to a second aspect of the present disclosure, there is provided a system, including: a memory configured to store computer-executable instructions; and one or more processors in communication with the memory and configured to execute the computer-executable instructions to: access characterization data of a feedstock, the characterization data including one or more spectra collected according to one or more spectroscopic methods; predict, using the characterization data, a set of constituent materials included in the feedstock; predict a material composition of the feedstock using the predicted set of constituent materials; identify, at least in part using the predicted material composition of the feedstock, one or more target products; generate a set of chemical reaction schemas enabling a conversion of at least part of the feedstock into the one or more target products; store identifications of the material composition of the feedstock, the one or more target products, and the set of chemical reaction schemas in a data store; and direct a portion of the feedstock to a materials recycling facility configured to convert the portion of the feedstock to at least one target product of the one or more target products.

[0009] Disclosed herein is a computer-readable storage medium for storing computer-executable instructions that, when executed, cause one or more processors of a computer system to perform one or more aspects of the method described above.

BRIEF DESCRIPTION OF THE DRAWINGS

[0010] FIG. 1 illustrates an example technique for managing reuse of molecular components of a feedstock, in accordance with some embodiments of the present disclosure.

CLAIMS

1. A method comprising:

accessing characterization data of a feedstock, the characterization data comprising one or more spectra collected according to one or more spectroscopic methods;

predicting, using the characterization data, a set of constituent materials included in the feedstock;

predicting a material composition of the feedstock using the predicted set of constituent materials;

identifying, at least in part using the predicted material composition of the feedstock, one or more target products;

generating a set of chemical reaction schemas enabling a conversion of at least part of the feedstock into the one or more target products;

storing identifications of the material composition of the feedstock, the one or more target products, and the set of chemical reaction schemas in a data store; and

directing a portion of the feedstock to a materials recycling facility configured to convert the portion of the feedstock to at least one target product of the one or more target products.

2. The method of claim 1, further comprising:

identifying one or more inputs to a fitness function, the one or more inputs describing a chemical reaction scheme of the set of chemical reaction schemas;

generating an output of the fitness function using the one or more inputs; and

selecting an implementation scheme from the set of chemical reaction schemas according to the fitness function, the one or more inputs, and the one or more target products.

3. The method of claim 1 or 2, wherein identifying the one or more target products comprises:

accessing inventory information describing a set of products; and

identifying an incomplete subset of the set of products as the one or more target products using the inventory information.

4. The method of any one of claims 1 to 3, wherein predicting the set of constituent materials included in the feedstock comprises:

accessing a library of spectra and associated metadata corresponding to the one or more spectroscopic methods;

identifying a band in the one or more spectra of the characterization data; and

matching the band to a spectrum of the library of spectra to predict a constituent material of the set of constituent materials.

5. The method of any one of claims 1 to 4, wherein generating the set of chemical reaction schemas comprises:

accessing a chemical reaction inventory, the chemical reaction inventory comprising representations of chemical reactions describing a conversion of the feedstock to a target product of the one or more target products; and

populating the set of chemical reaction schemas from the chemical reaction inventory.

6. The method of any one of claims 1 to 5, wherein generating the set of chemical reaction schemas comprises:

simulating a first constituent reaction of a chemical reaction scheme of the set of chemical reaction schemas using a machine learning model;

estimating an output of a reward function, with an output of the machine learning model serving as an input to the reward function; and

estimating a maximum of the reward function by modifying an input to the machine learning model, wherein the input is an output from a second constituent reaction preceding the first constituent reaction in the chemical reaction scheme.

7. A system, comprising:

a memory configured to store computer-executable instructions; and

one or more processors in communication with the memory and configured to execute the computer-executable instructions to:

access characterization data of a feedstock, the characterization data comprising one or more spectra collected according to one or more spectroscopic methods;

predict, using the characterization data, a set of constituent materials included in the feedstock;

predict a material composition of the feedstock using the predicted set of constituent materials;

identify, at least in part using the predicted material composition of the feedstock, one or more target products;

generate a set of chemical reaction schemas enabling a conversion of at least part of the feedstock into the one or more target products;

store identifications of the material composition of the feedstock, the one or more target products, and the set of chemical reaction schemas in a data store; and

direct a portion of the feedstock to a materials recycling facility configured to convert the portion of the feedstock to at least one target product of the one or more target products.

8. The system of claim 7, wherein executing the computer-executable instructions further causes the one or more processors to:

identifying one or more inputs to a fitness function, the one or more inputs describing a chemical reaction scheme of the set of chemical reaction schemas;

generating an output of the fitness function using the one or more inputs; and

selecting an implementation scheme from the set of chemical reaction schemas according to the fitness function, the one or more inputs, and the one or more target products.

9. The system of claim 7 or 8, wherein identifying the one or more target products comprises:

accessing inventory information describing a set of products; and

identifying an incomplete subset of the set of products as the one or more target products using the inventory information

10. The system of any one of claims 7 to 9, wherein predicting the set of constituent materials included in the feedstock comprises:

accessing a library of spectra and associated metadata corresponding to the one or more spectroscopic methods;

identifying a band in the one or more spectra of the characterization data; and

matching the band to a spectrum of the library of spectra to predict a constituent material of the set of constituent materials.

11. The system of any one of claims 7 to 10, wherein generating the set of chemical reaction schemas comprises:

accessing a chemical reaction inventory, the chemical reaction inventory comprising representations of chemical reactions describing a conversion of the feedstock to a target product of the one or more target products; and

populating the set of chemical reaction schemas from the chemical reaction inventory.

12. The system of any one of claims 7 to 11, wherein generating the set of chemical reaction schemas comprises:

simulating a first constituent reaction of a chemical reaction scheme of the set of chemical reaction schemas using a machine learning model;

estimating an output of a reward function, with an output of the machine learning model serving as an input to the reward function; and

estimating a maximum of the reward function by modifying an input to the machine learning model, wherein the input is an output from a second constituent reaction preceding the first constituent reaction in the chemical reaction scheme.