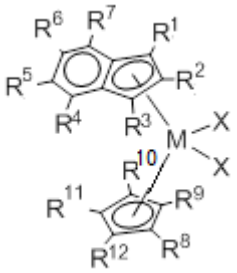


Formula I

[0010] where each of $R_1$ to $R_{12}$ is independently a $C_1$ to $C_{20}$ alkyl, aryl or aralkyl group, or a hydrogen, where at least one of $R_4$ to $R_7$ is not a hydrogen, where M is titanium, zirconium or hafnium, and where each X is independently a halide, $C_1$ to $C_{20}$ alkyl, aralkyl or hydrogen. It is noted that any of the adjacent R-groups may combine to form a ring, as described herein.

[0010a] In one aspect, the present disclosure refers to a polymerization catalyst, the polymerization catalyst comprising a metallocene catalyst of Formula I:



(Formula I)

wherein each of $R^1$ to $R^{12}$ is independently a $C_1$ to $C_{20}$ alkyl, aryl or aralkyl group, a hydrogen, wherein at least one of $R^4$ to $R^7$ is not a hydrogen, wherein M is a Group 4 metal, wherein, each X is independently a halide, $C_1$ to $C_{20}$ alkyl, aralkyl or hydrogen, and wherein:

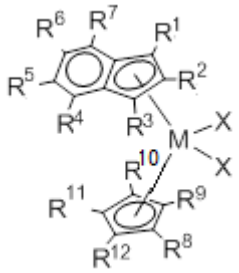
$R^5$ and $R^6$ of Formula I together form a cycloalkyl group; or

each of $R^7$ and $R^4$ of Formula I is independently a $C_1$ to $C_{20}$ alkyl and each of $R^1$, $R^2$, $R^3$, $R^5$ and $R^6$ of Formula I is a hydrogen.

[0011] The present disclosure provides polyethylene composition comprising polyethylene formed in a single reactor via a polymerization catalyst comprising a new metallocene catalyst of the Formula I, as described above.

[0011a] In another aspect, the present disclosure refers to a polyethylene composition comprising polyethylene formed in a single reactor via a polymerization

catalyst comprising a metallocene catalyst having improved ethylene enchainment of the formula:




(Formula I)

wherein each of $R^1$ to $R^{12}$ is independently a $C_1$ to $C_{20}$ alkyl, aryl or aralkyl group, or a hydrogen, wherein at least one of $R^4$ to $R^7$ is not a hydrogen, wherein M is a Group 4 metal, wherein, each X is independently a halide, $C_1$ to $C_{20}$ alkyl, aralkyl or hydrogen, and wherein:

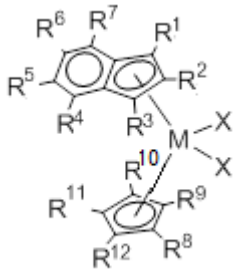
$R^5$ and $R^6$ of Formula I together form a cycloalkyl group; or

each of $R^7$ and $R^4$ of Formula I is independently a $C_1$ to $C_{20}$ alkyl and each of $R^1$, $R^2$, $R^3$, $R^5$ and $R^6$ of Formula I is a hydrogen.

[0012] The present disclosure provides methods of producing polyethylene, the method comprising polymerizing ethylene in a reactor in presence of a polymerization catalyst to form the polyethylene, where the polymerization catalyst comprises a new metallocene catalyst of Formula I, as described above.

[0012a] In yet another aspect, the present disclosure refers to a method of producing polyethylene having improved ethylene enchainment, the method comprising:

polymerizing ethylene in a reactor in presence of a polymerization catalyst to form the polyethylene, wherein the polymerization catalyst comprises a metallocene catalyst of Formula I:




(Formula I)

wherein each of $R^1$ to $R^{12}$ is independently a $C_1$ to $C_{20}$ alkyl, aryl or aralkyl group, or a hydrogen, wherein at least one of $R^4$ to $R^7$ is not a hydrogen, wherein M is a Group 4 metal, wherein, each X is independently a halide, $C_1$ to $C_{20}$ alkyl, aralkyl or hydrogen, and wherein:

$R^5$ and $R^6$ of Formula I together form a cycloalkyl group; or

each of $R^7$ and $R^4$ of Formula I is independently a $C_1$ to $C_{20}$ alkyl and each of $R^1$, $R^2$, $R^3$, $R^5$ and $R^6$ of Formula I is a hydrogen.

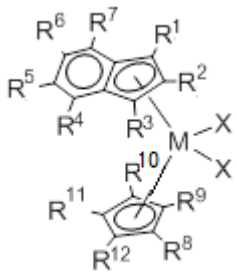
[0013] The above summary of the present disclosure is not intended to describe each disclosed example or every implementation of the present disclosure. The description that follows more particularly exemplifies illustrative examples. In several places throughout the application, guidance is provided through lists of examples, which examples can be used in various combinations. In each instance, the recited list serves only as a representative group and should not be interpreted as an exclusive list.

## Detailed Description

[0014] Polymerization catalysts, polyethylene compositions formed via polymerization catalysts, and methods of producing polyethylene employing polymerization catalysts are described herein. In general, the present techniques are directed to the new metallocene catalysts of Formula I that improves polymerization economics and gives desirable polymer properties. For instance, the polymerization catalyst including the new metallocene of Formula I can be employed in a single reactor

What is claimed:

1. A polymerization catalyst, the polymerization catalyst comprising a metallocene catalyst of Formula I:




(Formula I)

wherein each of $R^1$ to $R^{12}$ is independently a $C_1$ to $C_{20}$ alkyl, aryl or aralkyl group, a hydrogen, wherein at least one of $R^4$ to $R^7$ is not a hydrogen, wherein M is a Group 4 metal, wherein, each X is independently a halide, $C_1$ to $C_{20}$ alkyl, aralkyl or hydrogen, and wherein:

$R^5$ and $R^6$ of Formula I together form a cycloalkyl group; or

each of $R^7$ and $R^4$ of Formula I is independently a $C_1$ to $C_{20}$ alkyl and each of $R^1$, $R^2$, $R^3$, $R^5$ and $R^6$ of Formula I is a hydrogen.

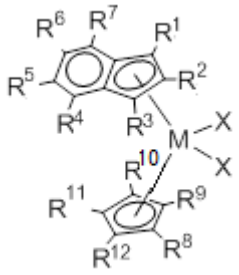
2. The polymerization catalyst of claim 1, wherein each of $R^9$, $R^{10}$, $R^{11}$ and $R^{12}$ of Formula I is a hydrogen.

3. The polymerization catalyst of claim 1, wherein the cycloalkyl group further comprises cyclohexyl-1,1,4,4-tetramethyl.

4. The polymerization catalyst of claim 1, wherein the $R^8$ of Formula I is a $C_1$ to $C_{20}$ alkyl; or a $C_1$ to $C_3$ alkyl.

5. The polymerization catalyst of claim 1, wherein M of Formula I further comprises titanium, zirconium or hafnium.

6. A polyethylene composition comprising polyethylene formed in a single reactor via a polymerization catalyst comprising a metallocene catalyst having improved ethylene enchainment of the formula:




(Formula I)

wherein each of $R^1$ to $R^{12}$ is independently a $C_1$ to $C_{20}$ alkyl, aryl or aralkyl group, or a hydrogen, wherein at least one of $R^4$ to $R^7$ is not a hydrogen, wherein M is a Group 4 metal, wherein, each X is independently a halide, $C_1$ to $C_{20}$ alkyl, aralkyl or hydrogen, and wherein:

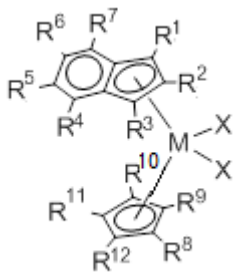
$R^5$ and $R^6$ of Formula I together form a cycloalkyl group; or

each of $R^7$ and $R^4$ of Formula I is independently a $C_1$ to $C_{20}$ alkyl and each of $R^1$, $R^2$, $R^3$, $R^5$ and $R^6$ of Formula I is a hydrogen.

7. The polyethylene composition of claim 6, wherein the polyethylene has a weight average molecular weight from 5,000 to 250,000 grams/mole (g/mol); or the polyethylene having the improved ethylene enchainment has a melt temperature of from 90 degrees Celsius to 136 degrees Celsius.

8. A method of producing polyethylene having improved ethylene enchainment, the method comprising:

polymerizing ethylene in a reactor in presence of a polymerization catalyst to form the polyethylene, wherein the polymerization catalyst comprises a metallocene catalyst of Formula I:




(Formula I)

wherein each of $R^1$ to $R^{12}$ is independently a $C_1$ to $C_{20}$ alkyl, aryl or aralkyl group, or a hydrogen, wherein at least one of $R^4$ to $R^7$ is not a hydrogen, wherein M is a Group 4 metal, wherein, each X is independently a halide, $C_1$ to $C_{20}$ alkyl, aralkyl or hydrogen, and wherein:

$R^5$ and $R^6$ of Formula I together form a cycloalkyl group; or

each of $R^7$ and $R^4$ of Formula I is independently a $C_1$ to $C_{20}$ alkyl and each of $R^1$, $R^2$, $R^3$, $R^5$ and $R^6$ of Formula I is a hydrogen.