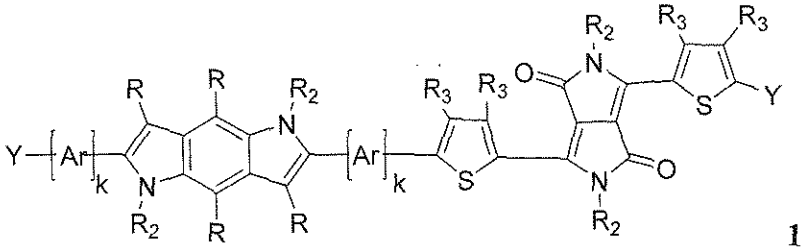
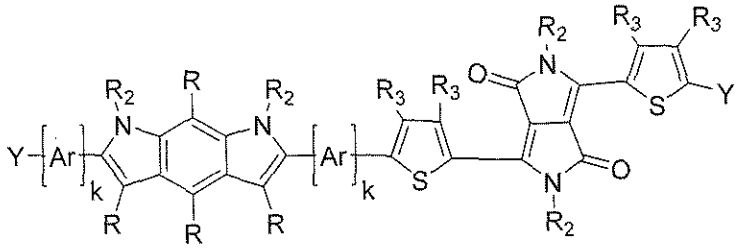
Summary

[0006] Embodiments comprise a rationally designed family of compounds and polymers comprising optionally-substituted dihydropyrroloindoles ("DHPI"), dipyrrolothiophenes or fused pyrroles (all generally referred to as "pyrrole groups" herein) bridged to optionally substituted diketopyrrolopyrroles ("DPP"). The materials have advantages over DPP alone in that they are soluble in non-chlorinated solvents, efficiently synthesized, and show very high mobilities in non-chlorinated solvents. Further, the compounds are relatively easy to modify and substituents can be introduced to multiple positions which allows for fine tuning material packing behaviors.

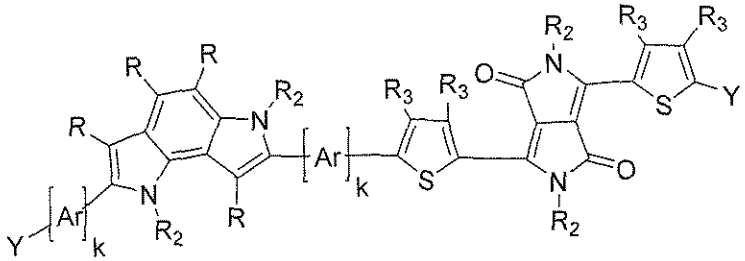
[0007] A first aspect~~embodiment~~ comprises a compound of formula:



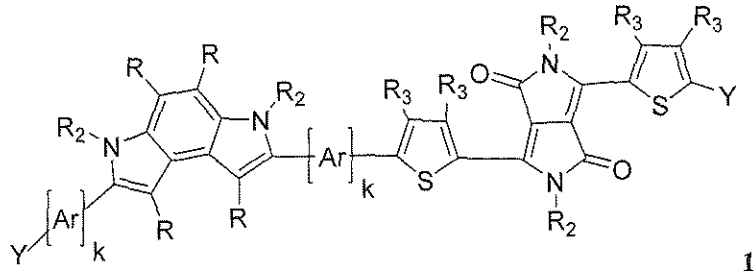
1a



1b



1c



1d

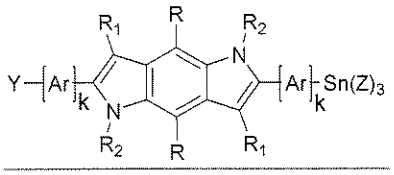
compound comprises **2**. In some embodiments, X is NR_1, PR_1, AsR_1, Sb, O, S, Se, or Te; and each R, R_1, R_2, and R_3 is independently H, halo, optionally substituted C_1-C_{40} alkyl, optionally substituted aralkyl, alkoxy, alkylthio, optionally substituted C_2-C_{40} alkenyl, optionally substituted C_2-C_{40} alkynyl, aminocarbonyl, acylamino, acyloxy, optionally substituted aryl, aryloxy, optionally substituted amino, carboxyalkyl, optionally substituted cycloalkyl, optionally substituted cycloalkenyl, halo, acyl, optionally substituted heteroaryl, optionally substituted heteroaralkyl, heteroaryloxy, optionally substituted heterocyclyl, thiol, alkylthio, heteroarylthiol, optionally substituted sulfoxide, or optionally substituted sulfone.

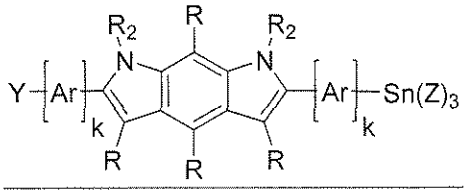
[0009] In other embodiments, each R, R_1, R_2, and R_3 is independently H, halo, optionally substituted C_1-C_{20} alkyl, optionally substituted aralkyl, alkoxy, alkylthio, optionally substituted C_2-C_{20} alkenyl, optionally substituted C_2-C_{20} alkynyl, optionally substituted cycloalkyl, optionally substituted cycloalkenyl, halo, optionally substituted heterocyclyl, or an optionally substituted aryl or optionally substituted heteroaryl from the group consisting of phenyl, thiophenyl, furanyl, pyrrolyl, imidazolyl, triazolyl, oxaxolyl, thiazolyl, pyridinyl, pyrimidinyl, triazinyl, naphthalenyl, isoquinolinyl, quinolinyl, or naphthyridinyl. In some embodiments, each R_2 is independently H, halo, or optionally substituted C_1-C_{20} alkyl.

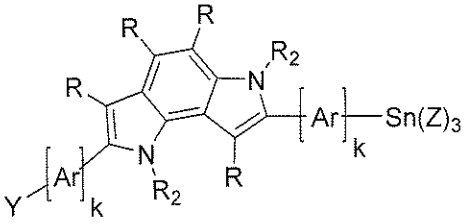
[0010] In particular embodiments, it is advantageous to have at least one or more of R, R_2, or R_3 independently be an optionally substituted C_1-C_{20} alkyl, and in particular an optionally substituted branched C_1-C_{20} alkyl. Particular embodiments may have optionally substituted C_1-C_{20} alkyl groups only on one or more R_2 groups, or alternatively only on one or more R groups.

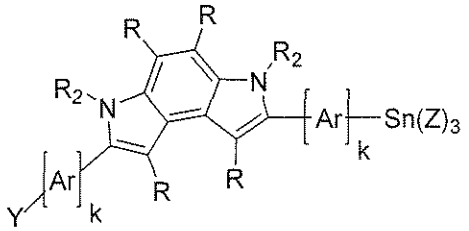
[0011] In some embodiments, the compound comprises **1a**, **1b**, **1c**, **1d**, **1e** or **2**, and the hole reorganization energy is less than 0.75 eV, less than 0.65, less than 0.5, less than 0.4, or less than 0.35 eV. In some embodiments, the hole reorganization energy is from about 0.05 to about 0.75, about 0.05 to about 0.65, about 0.05 to about 0.5, about 0.05 to about 0.04 or about 0.05 to about 0.35 eV.

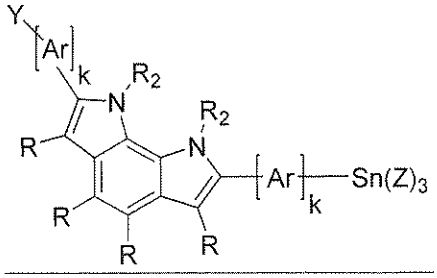
[0011a] In another aspect, there is provided a method of making a compound as defined above, the method comprising reacting a compound of structure:

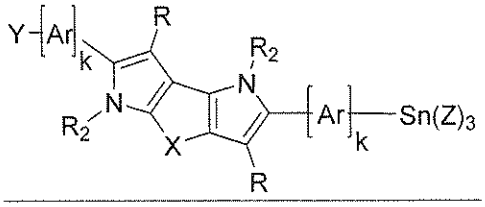




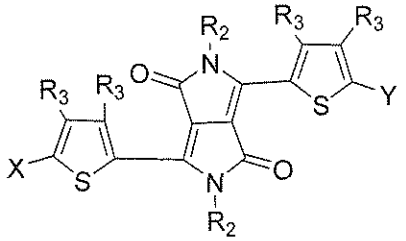






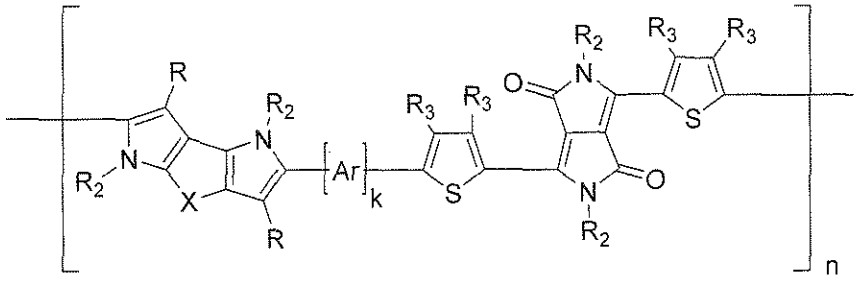


with a compound of structure:



where X is halo and Z is H or an optionally substituted alkyl.

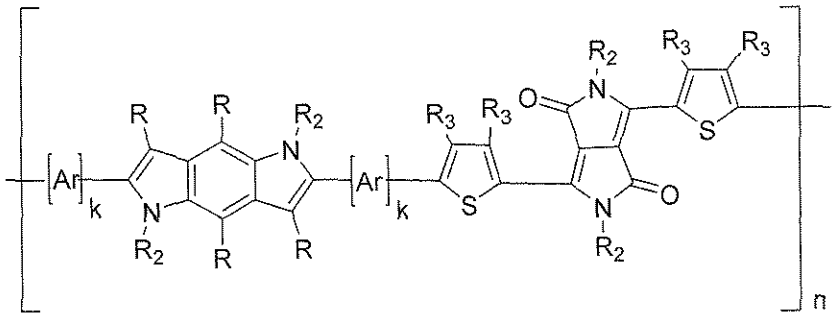
[0012] Another embodiment comprises a polymer of formula:



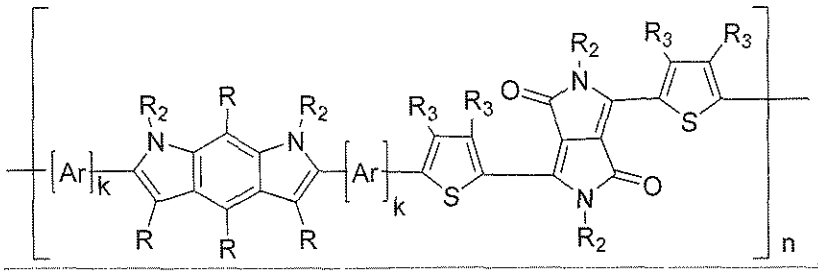
2'

wherein Ar is an optionally substituted aromatic or heteroaromatic group or conjugated group; k is an integer from 0 to 5 with the proviso that when k is 0, the structure results in a direct bond between the thiophene and diindole groups; n is an integer greater than zero; each X is independently NR_1, PR_1, AsR_1, Sb, O, S, Te, or Se, with the proviso that due to conjugation, X may be bonded to one or more additional R_1; each R, R_1, R_2, and R_3 is independently H, halo, optionally substituted C_1-C_{40} alkyl, optionally substituted aralkyl, alkoxy, alkylthio, optionally substituted C_2-C_{40} alkenyl, optionally substituted C_2-C_{40} alkynyl, aminocarbonyl, acylamino, acyloxy, optionally substituted aryl, aryloxy, optionally substituted amino, carboxyalkyl, optionally substituted cycloalkyl, optionally substituted cycloalkenyl, acyl, optionally substituted heteroaryl, optionally substituted heteroaralkyl, heteroaryloxy, optionally substituted heterocyclyl, thiol, alkylthio, heteroarylthiol, optionally substituted sulfoxide, or optionally substituted sulfone.

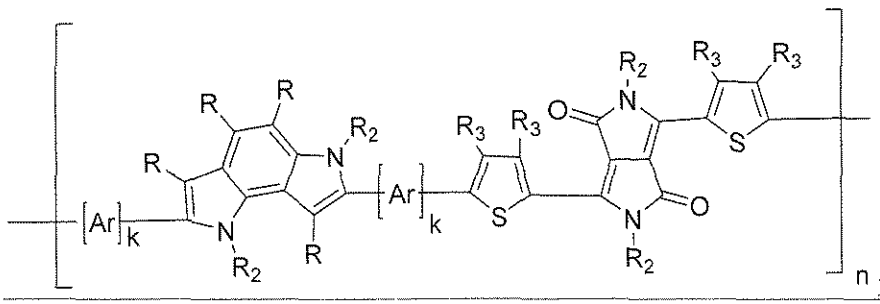
[0012a] In another aspect, there is provided a polymer comprising at least one moiety of formula:



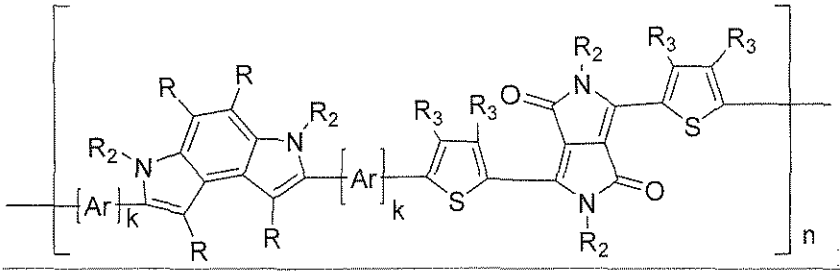
1a'



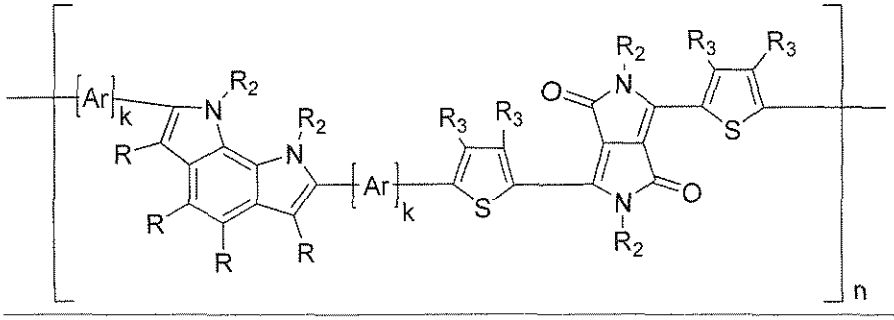
1b'



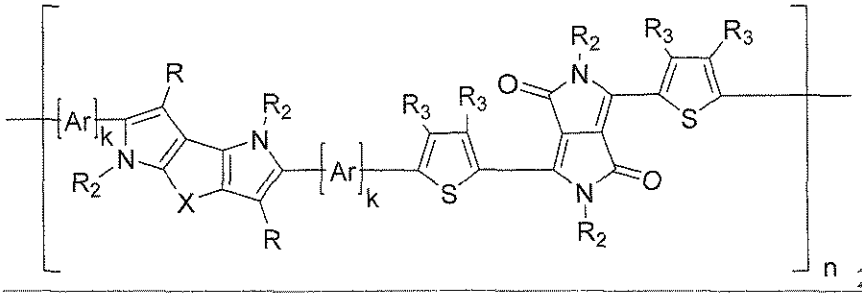
1e'



1d'



1e' or



2'

wherein n is an integer greater than zero; Ar is an optionally substituted aromatic or heteroaromatic group or conjugated group; k is an integer from 0 to 5 with the proviso that when k is 0, the structure results in a direct bond between the thiophene and pyrrole group; each X is independently NR_1, PR_1, AsR_1, Sb, O, S, Te, or Se, with the proviso that due to conjugation, X may be bonded to one or more additional R_1; and each R, R_1, R_2, and R_3 is independently H, halo, optionally substituted C_1-C_{40} alkyl, optionally substituted aralkyl, alkoxy, alkylthio, optionally substituted C_2-C_{40} alkenyl, optionally substituted C_2-C_{40} alkynyl, aminocarbonyl, acylamino, acyloxy, optionally substituted aryl, aryloxy, optionally substituted amino, carboxyalkyl, optionally substituted cycloalkyl, optionally substituted cycloalkenyl, acyl, optionally substituted

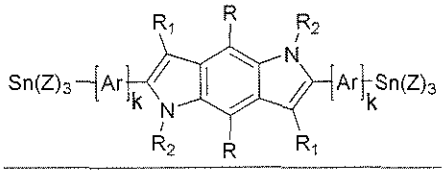
heteroaryl, optionally substituted heteroaralkyl, heteroaryloxy, optionally substituted heterocyclyl, thiol, alkylthio, heteroarylthiol, optionally substituted sulfoxide, or optionally substituted sulfone.

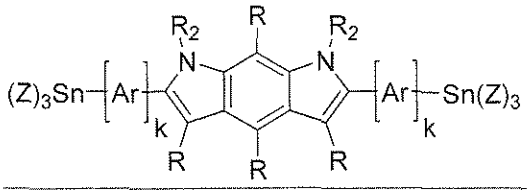
[0013] In some embodiments, the compound comprises **1a'** or **1b'**. In other embodiments, the compound comprises **1c', 1d',** or **1e'**. In still other embodiments, the compound comprises **2'**. In some embodiments, for **1a', 1b', 1c', 1d', 1e'**, or **2'**, X is NR_1, PR_1, AsR_1, Sb, O, S, Se, or Te, with the proviso that due to conjugation, X_1 may be bonded to one or more additional R_1; and each R, R_1, R_2, and R_3 is independently H, halo, optionally substituted C_1-C_{20} alkyl, optionally substituted aralkyl, alkoxy, alkylthio, optionally substituted C_2-C_{20} alkenyl, optionally substituted C_2-C_{20} alkynyl, aminocarbonyl, acylamino, acyloxy, optionally substituted aryl, aryloxy, optionally substituted amino, carboxyalkyl, optionally substituted cycloalkyl, optionally substituted cycloalkenyl, halo, acyl, optionally substituted heteroaryl, optionally substituted heteroaralkyl, heteroaryloxy, optionally substituted heterocyclyl, thiol, alkylthio, heteroarylthiol, optionally substituted sulfoxide, or optionally substituted sulfone.

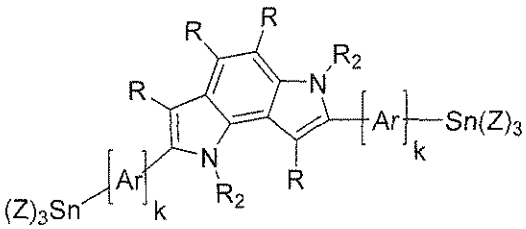
each Y is independently H, halo, trialkylsilane optionally substituted C_1-C_{20} alkyl, optionally substituted aralkyl, alkoxy, alkylthio, optionally substituted C_2-C_{20} alkenyl, optionally substituted C_2-C_{40} alkynyl, aminocarbonyl, acylamino, acyloxy, aryl, aryloxy, optionally substituted amino, carboxyalkyl, optionally substituted cycloalkyl, optionally substituted cycloalkenyl, halo, acyl, optionally substituted heteroaryl, optionally substituted heteroaralkyl, heteroaryloxy, optionally substituted heterocyclyl, thiol, alkylthio, heteroarylthiol, optionally substituted sulfoxide, optionally substituted sulfone, OSO-alkyl, Mg-halo, Zn-halo, $Sn(alkyl)_3$, SnH_3, $B(OH)_2$, $B(alkoxy)_2$, or OTs.

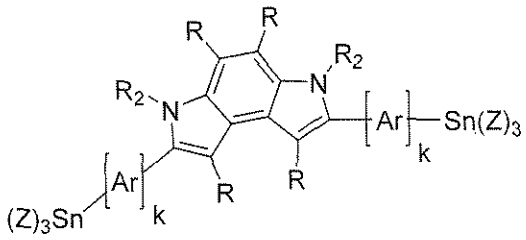
[0019] Another embodiment comprises a device comprising compound **1a**, **1b**, **1c**, **1d**, **1e**, or **2** or polymer **1a'**, **1b'**, **1c'**, **1d'**, **1e'**, or **2'**.

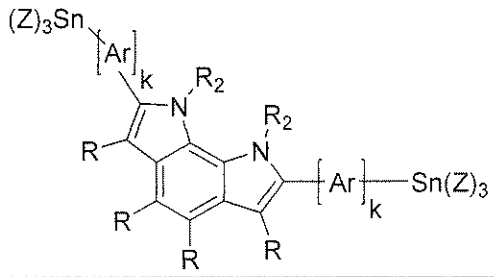
[0019a] In another aspect, there is provided a method of making the polymer as defined above, the method comprising reacting one or more compounds of formula:

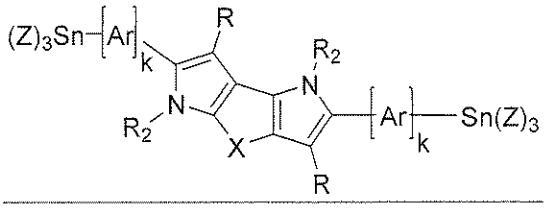




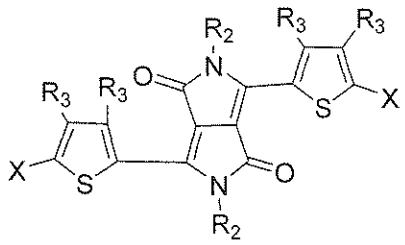








with one or more compounds of structure:



where X is halo and Z is H or an optionally substituted alkyl.

[0020] Additional features and advantages will be set forth in the detailed description which follows, and in part will be readily apparent to those skilled in the art from the description or recognized by practicing the embodiments as described in the written description and claims hereof, as well as in the appended drawings.

[0021] It is to be understood that both the foregoing general description and the following detailed description are merely exemplary, and are intended to provide an overview or framework for understanding.

Brief Description of the Drawings

[0022] The accompanying drawings are included to provide a further understanding, and are incorporated in and constitute a part of this specification.

[0023] **FIG. 1** is a graph of a simple mobility ranking metric based on linear combination of Neutral Dipole Moment and the inverse of the Reorganization Energy. Corresponding values for this metric have to be maximized for an optimal mobility property. Corning's previous polymer is at the Pareto Front 27 and is ranked lowest in this classification.

Detailed Description

[0024] Before the present materials, articles, and/or methods are disclosed and described, it is to be understood that the aspects described below are not limited to specific compounds, synthetic methods, or uses as such may, of course, vary. It is also to be understood that the terminology used herein is for the purpose of describing particular aspects only and is not intended to be limiting.