(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
30 January 2020 (30.01.2020)

WIPO | PCT

(10) International Publication Number
WO 2020/021008 A1

(51) International Patent Classification:
G06F 17/50 (2006.01)

(21) International Application Number:
PCT/EP2019/070038

(22) International Filing Date:
25 July 2019 (25.07.2019)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
62/711,018 27 July 2018 (27.07.2018) US

(71) Applicant: **TECHNISCHE UNIVERSITEIT EINDHOVEN** [NL/NL]; Den Dolech 2, 5612 AZ Eindhoven (NL).

(72) Inventors: **COEHOORN, Reinder;** Florapark 110, 5644 BZ Eindhoven (NL). **BOBBERT, Peter Arnold;** De Vroente 91, 5672 TV Nuenen (NL). **LIU, Feilong;** Julianastraat 1, 5611 HS Eindhoven (NL). **COTTAAR, Jeroen;** Palamedesweg 15, 5631 KT Eindhoven (NL).

(74) Agent: **FRKELLY;** 27 Clyde Road, Dublin, D04 F838 (IE).

(81) Designated States *(unless otherwise indicated, for every kind of national protection available)*: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BN, BR, BW, BY, BZ, CA, CH, CL, CN, CO, CR, CU, CZ, DE, DJ, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IR, IS, JO, JP, KE, KG, KH, KN, KP, KR, KW, KZ, LA, LC, LK, LR, LS, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PA, PE, PG, PH, PL, PT, QA, RO, RS, RU, RW, SA,

(54) Title: THREE-DIMENSIONAL MASTER EQUATION SIMULATIONS OF CHARGE-CARRIER TRANSPORT AND RECOMBINATION IN ORGANIC SEMICONDUCTOR MATERIALS AND DEVICES

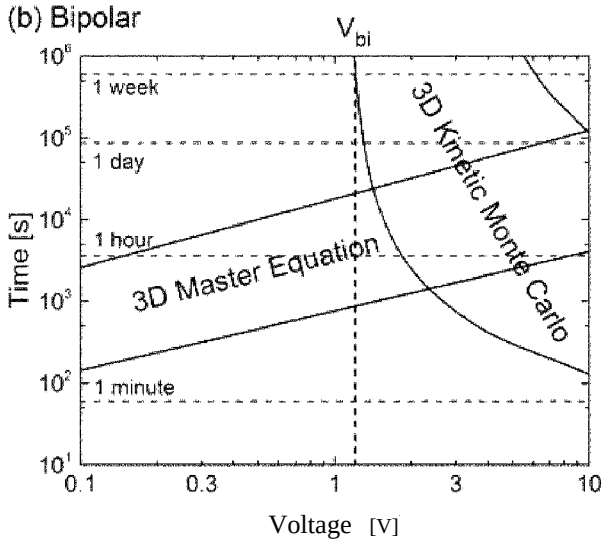

FIG. 1B

(57) Abstract: Three-dimensional master equation modeling for disordered semiconductor devices is provided. Charge transport is modeled as incoherent hopping between localized molecular states, and recombination is modeled as a nearest-neighbor process where an electron at a first location and a hole at a second location can recombine at either the first location or the second location. Here the first and second locations are any pair of nearest neighbor locations. We have found that this nearest neighbor recombination model performs substantially better than the conventional local recombination model where an electron and a hole must be at the same location to recombine. The recombination rate is modeled as a product of a prefactor Y, hopping rates and state occupancies. Importantly, we have found that sufficient simulation accuracy can be obtained by taking Y to be given by an empirically derived analytic expression.

WO 2020/021008 A1

[Continued on next page]