Javier Martinez-Salazar

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	A computer simulation of the effect of temperature on melt chain dimensions of random short chain branched polyethylene. Polymer, 2021, 225, 123772.	1.8	1
2	The Role of Key Amino Acids in the Antimicrobial Mechanism of a Bacteriocin Model Revealed by Molecular Simulations. Journal of Chemical Information and Modeling, 2021, 61, 6066-6078.	2.5	4
3	Organocatalyzed Polymerization of PET- <i>mb</i> -poly(oxyhexane) Copolymers and Their Self-Assembly into Double Crystalline Superstructures. Macromolecules, 2019, 52, 6834-6848.	2.2	15
4	Hydrodynamic and Electrophoretic Properties of Trastuzumab/HER2 Extracellular Domain Complexes as Revealed by Experimental Techniques and Computational Simulations. International Journal of Molecular Sciences, 2019, 20, 1076.	1.8	5
5	Predicting experimental results for polyethylene by computer simulation. European Polymer Journal, 2018, 99, 298-331.	2.6	47
6	Competition between supernucleation and plasticization in the crystallization and rheological behavior of PCL/CNT-based nanocomposites and nanohybrids. Journal of Polymer Science, Part B: Polymer Physics, 2017, 55, 1310-1325.	2.4	15
7	Mapping the Mechanical Properties of Poly(3-hydroxybutyrate-co-3-hydroxyvalerate) Banded Spherulites by Nanoindentation. Polymers, 2016, 8, 358.	2.0	6
8	New habits in branched polyethylene single crystals. European Polymer Journal, 2016, 80, 169-174.	2.6	5
9	A new insight into the conformation and melt dynamics of hydrogenated polybutadiene as revealed by computer simulations. Soft Matter, 2016, 12, 3929-3936.	1.2	8
10	Evidences of Changes in Surface Electrostatic Charge Distribution during Stabilization of HPV16 Virus-Like Particles. PLoS ONE, 2016, 11, e0149009.	1.1	5
11	The influence of short-chain branching on the morphology and structure of polyethylene single crystals. Journal of Polymer Science, Part B: Polymer Physics, 2015, 53, 1751-1762.	2.4	11
12	Molecular Dynamics Simulations for the Description of Experimental Molecular Conformation, Melt Dynamics, and Phase Transitions in Polyethylene. Macromolecules, 2015, 48, 5016-5027.	2.2	76
13	Study of the effect of the molecular architecture of the components on the melt rheological properties of polyethylene blends. Journal of Polymer Research, 2015, 22, 1.	1.2	5
14	Computer simulations of the early stages of crystal nucleation of linear and short chain branched polyethylene on carbon nanotubes. European Polymer Journal, 2014, 56, 194-204.	2.6	15
15	Strong influence of branching on the early stage of nucleation and crystal formation of fast cooled ultralong n-alkanes as revealed by computer simulation. European Polymer Journal, 2014, 50, 190-199.	2.6	22
16	Effect of short chain branching in molecular dimensions and Newtonian viscosity of ethylene/1-hexene copolymers: matching conformational and rheological experimental properties and atomistic simulations. Rheologica Acta, 2014, 53, 1-13.	1.1	17
17	Influence of Chain Branching and Molecular Weight on Melt Rheology and Crystallization of Polyethylene/Carbon Nanotube Nanocomposites. Macromolecules, 2014, 47, 5668-5681.	2.2	49
18	Exploring the dynamics and interaction of a full ErbB2 receptor and Trastuzumab-Fab antibody in a lipid bilayer model using Martini coarse-grained force field. Journal of Computer-Aided Molecular Design, 2014, 28, 1093-1107.	1.3	7

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19	3D-QSAR as a Tool for Understanding and Improving Single-Site Polymerization Catalysts. A Review. Organometallics, 2014, 33, 2944-2959.	1.1	56
20	Protein-Protein and Protein-Membrane Interactions Regarding the Erbb2/Trastuzumab-Fab Complexes. A Coarse-Grained Molecular Dynamics Description. Biophysical Journal, 2014, 106, 666a-667a.	0.2	1
21	Microstructure and properties of branched polyethylene: Application of a threeâ€phase structural model. Journal of Applied Polymer Science, 2013, 128, 1871-1878.	1.3	12
22	Effect of high molar mass species on linear viscoelastic properties of polyethylene melts. European Polymer Journal, 2013, 49, 2748-2758.	2.6	8
23	Conformational flexibility of the ErbB2 ectodomain and trastuzumab antibody complex as revealed by molecular dynamics and principal component analysis. Journal of Molecular Modeling, 2013, 19, 1227-1236.	0.8	8
24	Simulation of homology models for the extracellular domains (ECD) of ErbB3, ErbB4 and the ErbB2–ErbB3 complex in their active conformations. Journal of Molecular Modeling, 2013, 19, 931-941.	0.8	8
25	Bacteriocin AS-48 binding to model membranes and pore formation as revealed by coarse-grained simulations. Biochimica Et Biophysica Acta - Biomembranes, 2013, 1828, 2524-2531.	1.4	37
26	Structural Insights on the Plant Salt-Overly-Sensitive 1 (SOS1) Na+/H+ Antiporter. Journal of Molecular Biology, 2012, 424, 283-294.	2.0	49
27	Assessment of the Intrinsic Conformational Preferences of Dipeptide Amino Acids in Aqueous Solution by Combined Umbrella Sampling/MBAR Statistics. A Comparison with Experimental Results. Journal of Physical Chemistry B, 2012, 116, 469-475.	1.2	11
28	Following the Crystallization Process of Polyethylene Single Chain by Molecular Dynamics: The Role of Lateral Chain Defects. Macromolecular Symposia, 2012, 312, 97-107.	0.4	17
29	Polymerization Activity Prediction of Zirconocene Single-Site Catalysts Using 3D Quantitative Structure–Activity Relationship Modeling. Organometallics, 2012, 31, 1673-1679.	1.1	26
30	Assessment of entanglement features and dynamics from atomistic simulations and experiments in linear and short chain branched polyolefins. Soft Matter, 2012, 8, 6256.	1.2	17
31	A Curtin–Hammett mechanism for the copolymerization of ethylene and methyl acrylate monomer using a PymNox nickel catalyst as revealed by DFT computational studies. Journal of Molecular Modeling, 2012, 18, 515-523.	0.8	4
32	Effect of molecular weight distribution on Newtonian viscosity of linear polyethylene. Rheologica Acta, 2012, 51, 81-87.	1.1	23
33	Water-Mediated Conformations of the Alanine Dipeptide as Revealed by Distributed Umbrella Sampling Simulations, Quantum Mechanics Based Calculations, and Experimental Data. Journal of Physical Chemistry B, 2011, 115, 4880-4886.	1.2	33
34	Eliminating sharkskin distortion in polyethylene extrusion via a molecular route. Journal of Rheology, 2011, 55, 855-873.	1.3	11
35	Dissimilar interaction of CB1/CB2 with lipid bilayers as revealed by molecular dynamics simulation. Physical Chemistry Chemical Physics, 2011, 13, 3660-3668.	1.3	6
36	A three-phase microstructural model to explain the mechanical relaxations of branched polyethylene: a DSC, WAXD and DMTA combined study. Colloid and Polymer Science, 2011, 289, 257-268.	1.0	24

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37	Molecular architecture and linear viscoelasticity of homogeneous ethylene/styrene copolymers. Rheologica Acta, 2011, 50, 207-220.	1.1	7
38	Size and conformational features of ErbB2 and ErbB3 receptors: a TEM and DLS comparative study. European Biophysics Journal, 2011, 40, 835-842.	1.2	11
39	Computer modeling of the crystallization process of singleâ€chain ethylene/1â€hexene copolymers from dilute solutions. Journal of Polymer Science, Part B: Polymer Physics, 2011, 49, 421-430.	2.4	21
40	Role of the interface in the meltâ€rheology properties of linear lowâ€density polyethylene/lowâ€density polyethylene blends: Effect of the molecular architecture of the dispersed phase. Journal of Applied Polymer Science, 2011, 119, 3217-3226.	1.3	8
41	Density functional study for the polymerization of ethylene monomer using a new nickel catalyst. Journal of Polymer Science Part A, 2010, 48, 1160-1165.	2.5	8
42	The role of the interface in melt linear viscoelastic properties of LLDPE/LDPE blends: Effect of the molecular architecture of the matrix. Journal of Applied Polymer Science, 2009, 114, 420-429.	1.3	12
43	Rheology, Processing, Tensile Properties, and Crystallization of Polyethylene/Carbon Nanotube Nanocomposites. Macromolecules, 2009, 42, 4719-4727.	2.2	153
44	Theoretical Study on a Multicenter Model Based on Different Metal Oxidation States for the Bis(imino)pyridine Iron Catalysts in Ethylene Polymerization. Organometallics, 2009, 28, 5889-5895.	1.1	43
45	Viscoelasticity and macromolecular topology in single-site catalyzed polyethylene. Journal of Materials Science, 2008, 43, 1745-1748.	1.7	5
46	Structure and Physical Properties of Polyethylenes obtained from Dual Catalysis Process. Polymer Bulletin, 2008, 60, 331-342.	1.7	9
47	Entanglement network and relaxation temperature dependence of singleâ€site catalyzed ethylene/1â€hexene copolymers. Journal of Applied Polymer Science, 2008, 109, 1564-1569.	1.3	13
48	Highly active ethylene/hydroxyl comonomers copolymerization using metallocene catalysts. Journal of Applied Polymer Science, 2008, 109, 1529-1534.	1.3	10
49	Three-dimensional modelling of flow curves in co-rotating twin-screw extruder elements. Journal of Materials Processing Technology, 2008, 197, 221-224.	3.1	24
50	Estradiol supplementation during the luteal phase of IVF-ICSI patients: a randomized, controlled trial. Fertility and Sterility, 2008, 90, 2190-2195.	0.5	33
51	Entanglement Relaxation Time in Polyethylene: Simulation versus Experimental Data. Macromolecules, 2008, 41, 2959-2962.	2.2	46
52	On the Nature of the Active Site in bis(imino)Pyridyl Iron, a Catalyst for Olefin Polymerization. Journal of Physical Chemistry C, 2008, 112, 5023-5028.	1.5	34
53	Proposed Polymerization Termination Mechanism for 3-R-Indenyl <i>ansa</i> -Zirconocenes (R =) Tj ETQq1 1 0.78 7413-7415.	4314 rgBT 2.2	/Overlock 1 4
54	Molecular structure and properties of ethyleneâ€ <i>co</i> â€styrene polymers obtained from [norbornaneâ€7,7â€bis(1â€indenyl)]titanium dichloride catalyst system. Journal of Applied Polymer Science, 2007, 106, 1421-1430.	1.3	5

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55	QSAR model for ethylene polymerisation catalysed by supported bis(imino)pyridine iron complexes. Polymer, 2007, 48, 7672-7678.	1.8	30
56	The unit cell expansion of branched polyethylene as detected by Raman spectroscopy: an experimental and simulation approach. Journal of Materials Science, 2007, 42, 1046-1049.	1.7	23
57	3D-QSAR study of ansa-metallocene catalytic behavior in ethylene polymerization. Polymer, 2007, 48, 4663-4674.	1.8	30
58	meso-[Norbornane-7,7-bis(indenyl)]titanium Dichloride:Â A Highly Active Catalyst for Ethyleneâ^'Styrene Copolymerization. Macromolecules, 2006, 39, 7479-7482.	2.2	21
59	Isomeric effect of the Et(H4Ind)2Zr(CH3)2 catalyst on the copolymerization of ethylene and styrene: A computational study. Journal of Polymer Science Part A, 2006, 44, 4752-4761.	2.5	10
60	Melt flow index on high molecular weight polyethylene: A comparative study of experiments and simulation. Journal of Materials Processing Technology, 2006, 174, 171-177.	3.1	13
61	Viscoelastic behaviour during the crystallisation of isotactic polypropylene. Journal of Materials Science, 2006, 41, 3899-3905.	1.7	5
62	Rheological behaviour of LDPE/EVAc blends. II. Linear viscoelasticity and extrusion properties. Journal of Materials Science, 2006, 41, 4814-4822.	1.7	6
63	A QM/MM study of the ethylene and styrene insertion process into the ion pair [Me2Si(C5Me4)(NtBu)Ti(CH2CH2CH3)]+[î¼-Me–Al(Me)2–(AlOMe)6Me]â^'. Polymer, 2006, 47, 883-896.	1.8	10
64	Synthesis and properties of ethylene/styrene copolymers produced by metallocene catalysts. Journal of Applied Polymer Science, 2006, 102, 3420-3429.	1.3	10
65	Processability of a metallocene-catalyzed linear PE improved by blending with a small amount of UHMWPE. Journal of Polymer Science, Part B: Polymer Physics, 2005, 43, 2963-2971.	2.4	29
66	An experimental and computational evaluation of ethylene/styrene copolymerization with a homogeneous single-site titanium(IV)-constrained geometry catalyst. Journal of Polymer Science Part A, 2005, 43, 711-725.	2.5	28
67	Ethylene-styrene copolymerization with constrained geometry catalysts: A density functional study. Journal of Chemical Physics, 2005, 122, 074901.	1.2	17
68	Structureâ^'Activity Relationship Study of the Metallocene Catalyst Activity in Ethylene Polymerization. Organometallics, 2005, 24, 5095-5102.	1.1	58
69	3D-QSAR analysis of metallocene-based catalysts used in ethylene polymerisation. Polymer, 2004, 45, 2061-2072.	1.8	55
70	Ethylene/styrene copolymerisation by homogeneous metallocene catalysts: experimental and molecular simulations using rac-ethylenebis(tetrahydroindenyl)MCl2 [M=Ti,Zr] systems. Polymer, 2004, 45, 9029-9038.	1.8	21
71	Elimination of Extrudate Distortions in Metallocene-Catalyzed Polyethylene. Macromolecules, 2004, 37, 681-683.	2.2	11
72	Title is missing!. Journal of Materials Science, 2003, 38, 4757-4764.	1.7	14

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73	Rheological features and molecular architecture of polyethylenes. Polymer Bulletin, 2003, 50, 197-204.	1.7	11
74	Copolymerization of ethylene and styrene by homogeneous metallocene catalysts. 1. Theoretical studies with rac-ethylenebis-(tetrahydroindenyl)MCl2 [M=Ti, Zr] systems. Polymer, 2003, 44, 295-306.	1.8	21
75	Novel features of the rheological behaviour of metallocene catalysed atactic polypropylene. Polymer, 2003, 44, 1401-1407.	1.8	19
76	DFT study of hydrogenolysis as a chain transfer mechanism in olefin polymerisation catalysed by nickel-diimine-type catalysts. Polymer, 2003, 44, 2177-2186.	1.8	16
77	Computational studies of the Brookhart's type catalysts for ethylene polymerisation. Part 2: ethylene insertion and chain transfer mechanisms. Polymer, 2003, 44, 2169-2176.	1.8	20
78	Phase morphology and melt viscoelastic properties in blends of ethylene/vinyl acetate copolymer and metallocene-catalysed linear polyethylene. Polymer, 2003, 44, 2911-2918.	1.8	44
79	On the processability of metallocene-catalysed polyethylene: effects of blending with ethylene–vinyl acetate copolymer. Polymer, 2003, 44, 1589-1594.	1.8	17
80	Model linear metallocene-catalyzed polyolefins: Melt rheological behavior and molecular dynamics. Journal of Rheology, 2003, 47, 1505-1521.	1.3	21
81	Effect of long chain branching on linear-viscoelastic melt properties of polyolefins. E-Polymers, 2002, 2, .	1.3	24
82	A computational study of iron-based Gibson–Brookhart catalysts for the copolymerisation of ethylene and 1-hexene. Polymer, 2002, 43, 3635-3645.	1.8	28
83	A theoretical study of ethylene–styrene copolymerization by using half-sandwich Cp-based titanium catalysts. Polymer, 2002, 43, 7017-7026.	1.8	27
84	Title is missing!. Journal of Materials Science, 2002, 37, 3415-3421.	1.7	10
85	Ab initio study of ethylene insertion into M–C bonds of alkylamidinates complexes of group IV ({R′NCRNR′} 2 MCH 3 + , M=Zr, Ti, R=H, Ph and R′=H, SiMe 3). Polymer, 2001, 42, 7275-7284.	1.8	7
86	Rheological behaviour of LDPE/EVA-c blends. I. On the effect of vinyl acetate comonomer in EVA copolymers. Polymer, 2001, 42, 8093-8101.	1.8	25
87	Computational studies of the Brookhart's type catalysts for ethylene polymerization. 1. Effect of the active site conformations on the catalyst activities. Polymer, 2001, 42, 8019-8023.	1.8	12
88	New aspects on the rheological behaviour of metallocene catalysed polyethylenes. Polymer, 2001, 42, 9713-9721.	1.8	56
89	Effect of a second ethylene molecule on the insertion of ethylene in zirconocene catalyst systems: A QM semiempirical study. Journal of Polymer Science Part A, 2000, 38, 571-582.	2.5	23
90	Preparation and properties of terpolymers of ethylene, vinyl acetate and vinyl alcohol. Macromolecular Chemistry and Physics, 2000, 201, 1323-1328.	1.1	10

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91	Ab initio study of hydrogenolysis as a chain transfer mechanism in olefin polymerization catalyzed by metallocenes. Polymer, 2000, 41, 6161-6169.	1.8	22
92	The fine structure of metallocene-based linear polyethylenes: Part 1. A model grounded on molecular mobility. Polymer, 1999, 40, 4345-4352.	1.8	2
93	A theoretical study of the comonomer effect in the ethylene polymerization with zirconocene catalytic systems. Journal of Polymer Science Part A, 1998, 36, 1157-1167.	2.5	36
94	Effect of crystallization temperature on the cocrystallization of hydroxybutyrate/hydroxyvalerate copolymers. Polymer, 1997, 38, 913-919.	1.8	47
95	Crystallization kinetics and morphology of poly(propylene-stat-ethylene) fractions. Polymer, 1997, 38, 361-369.	1.8	55
96	Crystal structure and morphology of melt-crystallized poly(propylene-stat-ethylene) fractions. Polymer, 1997, 38, 371-377.	1.8	38
97	Fracture of binary blends of linear and branched polyethylene. Polymer, 1996, 37, 5123-5129.	1.8	13
98	On the melting behaviour of polymer single crystals in a mixture with a compatible oligomer: 2. Polyethylene/paraffin. Polymer, 1996, 37, 2367-2371.	1.8	6
99	Ab initio calculation of ethylene insertion in zirconocene catalyst systems: A comparative study between bridged and unbridged complexes. Polymer, 1996, 37, 1663-1667.	1.8	27
100	On the melting behaviour of polymer single crystals in a mixture with a compatible polymer: 1. Poly(vinylidene fluoride)/poly(methyl methacrylate) blends. Polymer, 1995, 36, 981-985.	1.8	20
101	Study of structural changes of tellurium thin films on polymer substrates by electrical measurements and transmission electron microscopy. Thin Solid Films, 1994, 245, 272-276.	0.8	4
102	Structural assessment of liquid-crystalline side-chain poly(vinyl ether)s: dependence on terminal group, orientation and temperature. Polymer, 1994, 35, 4041-4047.	1.8	9
103	Phase separation studies on poly(vinylidene fluoride) and poly(methyl methacrylate) quenched blends. Macromolecular Symposia, 1994, 78, 95-104.	0.4	8
104	On the Fine Structure of Shish-Kebabs in Injection Moulded Polyethylene. International Journal of Polymeric Materials and Polymeric Biomaterials, 1993, 21, 111-121.	1.8	16
105	On phase separation in high- and low-density polyethylene blends: 1. Melting-point depression analysis. Polymer, 1991, 32, 2984-2988.	1.8	38
106	On phase separation in high- and low-density polyethylene blends: 2. A working model. Polymer, 1991, 32, 2989-2991.	1.8	19
107	Conductive polyethylene-carbon black composites by elongational-flow injection molding Part 3. Study of the structure and morphology. Colloid and Polymer Science, 1989, 267, 409-413.	1.0	13
108	Physical ageing and glass transition in amorphous polymers as revealed by microhardness. Journal of Materials Science, 1989, 24, 2934-2938.	1.7	77

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109	Thermal expansion and spherulite cracking in 3-hydroxybutyrate/3-hydroxyvalerate copolymers. Journal of Materials Science Letters, 1989, 8, 490-492.	0.5	57
110	Phase changes in isotactic polypropylene measured by microhardness. Journal of Materials Science Letters, 1988, 7, 165-166.	0.5	39
111	Temperature dependence of microhardness in the 70/30 polyvinylidene fluoride-trifluorethylene copolymer: New structural aspects of the curie transition. Colloid and Polymer Science, 1988, 266, 41-45.	1.0	12
112	Microstructural changes in polyethylene-polypropylene blends as revealed by microhardness. Journal of Materials Science, 1988, 23, 862-866.	1.7	44
113	Conductive PE-carbon composites by elongation flow injection moulding. Journal of Materials Science, 1988, 23, 475-480.	1.7	28
114	Conducting injection moulded carbon black filled polyethylene. Makromolekulare Chemie Macromolecular Symposia, 1988, 20-21, 597-600.	0.6	2
115	Equilibrium and non-equilibrium melting of branched polyethylene relating to defect incorporation within crystals. Colloid and Polymer Science, 1987, 265, 239-245.	1.0	30
116	X-Ray diffraction study of lattice distortions in branched polyethylene rapidly quenched from the melt. Polymer Bulletin, 1987, 17, 23-30.	1.7	10
117	Percolation threshold of conductive polycarbonate/carbon composites as revealed by electron microscopy. Journal of Materials Science Letters, 1986, 5, 1065-1066.	0.5	37
118	The identification of the initial lamellar thickness of polyethylene crystals grown from the melt using synchrotron X-radiation. Journal of Materials Science, 1985, 20, 1616-1624.	1.7	37
119	The supercooling dependence of the initial fold length of polyethylene crystallized from the melt: unification of melt and solution crystallization. Journal of Materials Science, 1985, 20, 1625-1630.	1.7	98
120	Mechanical model on polyethylene blends as revealed by microhardness. Journal of Materials Science Letters, 1985, 4, 324-326.	0.5	16
121	Annealing effects in lamellar linear polyethylene as revealed by microhardness. Journal of Materials Science, 1985, 20, 834-838.	1.7	23
122	A study of diffractometer line shapes in melt crystallized polyethylene. Colloid and Polymer Science, 1984, 262, 361-365.	1.0	5
123	Studies on polyethylene crystallized at unusually high supercoolings: Fold length, habit, growth rate, epitaxy. Journal of Polymer Science, Polymer Physics Edition, 1984, 22, 1085-1096.	1.0	21
124	Transmission electron microscopy of polyamides. Journal of Materials Science Letters, 1984, 3, 693-694.	0.5	26
125	Lamellar structure in melt crystallized low density polyethylene. Polymer Bulletin, 1984, 12, 269.	1.7	11
126	Lamellar structure in melt crystallized low density polyethylene. Colloid and Polymer Science, 1983, 261, 412-416.	1.0	36

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127	Influence of chlorosulfonation on the surface mechanical properties of lamellar polyethylene. Polymer Bulletin, 1983, 10, 553-557.	1.7	13
128	Correlation of hardness and microstructure in unoriented lamellar polyethylene. Journal of Materials Science, 1983, 18, 1077-1082.	1.7	41
129	A new look at the crystallization of polyethylene. II. Crystallization from the melt at low supercoolings. Journal of Polymer Science, Polymer Physics Edition, 1982, 20, 1717-1732.	1.0	57
130	A new look at the crystallization of polyethylene. I. The initial fold length of melt-crystallized material. Journal of Polymer Science, Polymer Letters Edition, 1981, 19, 539-547.	0.4	38
131	On the inclusion of chain defects in the polyethylene lattice a statistical approach. Polymer Bulletin, 1980, 2, 163-167.	1.7	27
132	Long periods in melt crystallized polyethylene two coexisting structures?. Polymer Bulletin, 1980, 3-3, 7-12.	1.7	7
133	Influence of chain defects on the crystallization of polyethylene with reference to crystal size and perfection. Journal of Crystal Growth, 1980, 48, 283-294.	0.7	70
134	Distribution of chain defects and microstructure of melt crystallized polyethylene. Polymer, 1978, 19, 1094-1099.	1.8	64